TOPICAL REVIEW

Majorana fermions in semiconductor nanowires: fundamentals, modeling, and experiment

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Abstract

After a recent series of rapid and exciting developments, the long search for the Majorana fermion—the elusive quantum entity at the border between particles and antiparticles—has produced the first positive experimental results, but is not over yet. Originally proposed by E Majorana in the context of particle physics, Majorana fermions have a condensed matter analogue in the zero-energy bound states emerging in topological superconductors. A promising route to engineering topological superconductors capable of hosting Majorana zero modes consists of proximity coupling semiconductor thin films or nanowires with strong spin–orbit interaction to conventional s-wave superconductors in the presence of an external Zeeman field. The Majorana zero mode is predicted to emerge above a certain critical Zeeman field as a zero-energy state localized near the order parameter defects, namely, vortices for thin films and wire ends for the nanowire. These Majorana bound states are expected to manifest non-Abelian quantum statistics, which makes them ideal building blocks for fault-tolerant topological quantum computation. This review provides an update on the current status of the search for Majorana fermions in semiconductor nanowires by focusing on the recent developments, in particular the period following the first reports of experimental signatures consistent with the realization of Majorana bound states in semiconductor nanowire–superconductor hybrid structures. We start with a discussion of the fundamental aspects of the subject, followed by considerations on the realistic modeling, which is a critical bridge between theoretical predictions based on idealized conditions and the real world, as probed experimentally. The last part is dedicated to a few intriguing issues that were brought to the fore by the recent encouraging experimental advances.

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Topical Review

1. Introduction

In relativistic quantum mechanics spin-1/2 fermions are described by the solutions of the Dirac equation [1],

\[(i\gamma^\mu \partial_\mu - m)\psi = 0.\]  \( (1) \)

Here, \(\gamma^\mu (\mu = 0–3)\) is a set of \(4 \times 4\) matrices satisfying the anticommutation relations \([\gamma^\mu, \gamma^\nu] = 2g^{\mu\nu}\), where \(g^{\mu\nu}\) represents the Minkowski metric and \(\gamma^0\gamma^\nu \gamma^0 = \gamma^\nu\) \([2]\). In general, the matrices \(\gamma^\mu\) have complex elements, making equation (1) a set of coupled differential equations with complex coefficients. Thus, the general solution \(\psi(x)\) of equation (1) representing the fermion field is a complex bi-spinor that is not an eigenstate of the charge conjugation (CC) operator. Since charge conjugation, \(\psi \rightarrow \psi^*\), maps a particle into its antiparticle \([3]\), a complex solution of equation (1) represents a fermion that has a distinct anti-fermion, with the same mass and spin but opposite charge and magnetic moment, as its counterpart. Therefore, the field of a relativistic fermion that coincides with its own antiparticle, should it exist, is necessarily an eigenstate of CC that must be described by a real solution \(\psi(x)\) of equation (1). Real solutions of the Dirac equation are possible, provided one can find a suitable representation of the matrices \(\gamma^\mu\) characterized by purely imaginary non-zero matrix elements. Such a representation of the \(\gamma^\mu\) matrices that renders equation (1) purely real was found by Majorana in 1937 \([4]\). The real solutions \(\psi(x)\) correspond to charge-neutral fermions, known as Majorana fermions (MFs), representing particles that are their own antiparticles. Charge neutrality and the identification of the particle with its own antiparticle are not uncommon features among bosons—photons and \(\pi^0\)-mesons being two standard examples—but they are quite special among fermions. The neutron, for example, which is a charge-neutral fermion, has an antiparticle (the anti-neutron) that is distinguished from the neutron by the sign of its magnetic moment. Also, neutrinos produced in beta-decay are thought to be charge-neutral and have a small but non-zero rest mass (so that they cannot be Weyl fermions \([5]\), which are massless), but whether they are Dirac or Majorana fermions is still an unsettled question in particle physics.

While Majorana fermions have remained undetected in high-energy physics for almost 70 years, in the past decade they have made an emphatic entrance into the realm of condensed matter physics \([6–10]\). In this context, the term Majorana fermion does not refer to an elementary particle, but rather to quasiparticles corresponding to collective excitations of an underlying complicated many-body ground state. As shown by Read and Green \([11]\), in the so-called weak-pairing phase of a two-dimensional (2D) spinless \(p_x + ip_y\) superconductor (or superfluid), the quasiparticles satisfy an equation—the Bogoliubov–de Gennes (BdG) equation—that is similar to the Majorana form of the Dirac equation. These quasiparticles represent the solid state analogue of the Majorana fermions from high-energy physics and, in general, are characterized by a finite mass and have finite energy. However, in the context of the recent developments, the term ‘Majorana fermion’ has a slightly different meaning. In a superconductor, the spinless fermionic Bogoliubov quasiparticles satisfy particle–hole symmetry, \(\gamma^0 = \gamma_{-E}\), and, consequently, the zero-energy quasiparticles can be viewed as fermions that are identical to their own anti-quasiparticles, \(\gamma_0 = \gamma_0\). These BdG quasiparticles with zero excitation energy emerge as localized states bound to defects in the superconductor, where the order parameter amplitude vanishes, e.g., vortices and sample edges \([11]\). Furthermore, in two dimensions the quantum quasiparticles associated with these zero-energy bound states were shown to obey a form of quantum statistics known as non-Abelian statistics \([12, 13, 11, 14, 15]\). Exchanging two particles that obey non-Abelian statistics represents a non-commutative operation. Recently, the interest in the properties and the possible realization of non-Abelian zero-energy quasiparticles has increased dramatically, after they were proposed \([16]\) as possible building blocks for fault-tolerant topological quantum computation (TQC) \([6]\).

In this review, the terms ‘Majorana fermion’, ‘zero-energy Majorana state’, or ‘Majorana bound state’ refer to localized, charge-neutral, zero-energy states that occur at
defects and boundaries in topological superconductors. The creation operator for such a zero-energy state is a Hermitian second quantized operator $\gamma^\dagger = \gamma$ that anticommutes with other fermion operators and satisfies the relation $\gamma^2 = 1$. In a superconductor, a non-degenerate localized zero-energy eigenstate enjoys a form of topological protection that makes it immune to any local perturbation that does not close the superconducting gap. Such perturbations cannot move the state away from zero energy because of the particle–hole symmetry and the non-degeneracy condition. Since small perturbations to the BdG differential equation are not expected to change the total number of solutions, it necessarily follows that local perturbations (i.e., perturbations that do not couple pairs of MFs) leave the non-degenerate zero-energy eigenvalues unperturbed. This argument also implies that the zero-energy solutions are characterized by vanishing expectation values for any local physical observable, such as charge, mass, and spin. Otherwise, in the presence of a non-zero average, a local field that couples to the corresponding operator would shift the energy of the state. Thus, our use of the term ‘Majorana fermion’ is more restrictive than that in the particle physics literature: the MFs in this review are chargeless, massless, spinless, i.e., free of any internal quantum number, and obey non-Abelian statistics, while the MFs in particle physics satisfy standard Fermi statistics and, although charge-neutral, since they are eigenstates of the charge conjugation operator, can be massive and spin-full. Finally, as zero-energy MFs in solid state systems are topologically protected, they can be removed from zero energy only by driving the system through a topological quantum phase transition (TQPT) [17] characterized by the closing of the energy gap at the topological critical point, where the MFs become entangled with other gapless states [11].

Majorana fermions have recently been proposed in low-temperature solid state systems in the context of the fractional quantum Hall (FQH) effect [13, 11, 18, 12, 19–22], spinless chiral p-wave superconductors/superfluids [11, 23, 14, 21], in particular in strontium ruthenate, via the realization of the so-called half-quantum vortexes [24–26], heterostructures of topological insulators (TI) and superconductors [27–32], metallic surface states [33], metallic ferromagnet-cuprate high-$T_C$ superconductors [34], non-centro-symmetric superconductors [35–37], superconductors with odd-frequency pairing [38, 39], helical magnets [40], carbon nanotubes and graphene [41–44], spin–orbit-coupled ferromagnetic Josephson junctions [45], chains of magnetic atoms on a superconductor [46], and cold fermion systems with p-wave Feshbach resonance [47–50], or with s-wave Feshbach resonance plus artificially generated spin–orbit coupling and Zeeman splitting [51, 52]. It has also been shown that MFs can exist as quasiparticles localized in the topological defects and at the boundaries of a spin–orbit (SO)-coupled electron-doped semiconductor 2D thin film [53, 54] or 1D nanowire [54–56] with proximity-induced s-wave superconductivity and an externally induced Zeeman splitting. More recently, it was shown that similar mechanisms can lead to the emergence of MFs in hole-doped semiconductor structures [57, 58]. Although the physics responsible for the emergence of the zero-energy MFs is identical in both 2D and 1D systems (in 3D a similar mechanism produces a so-called Weyl superconductor/superfluid [59, 60] characterized by gapless, topologically protected, Weyl fermion nodes in the bulk), the nanowire setting has some experimental advantages, such as the option of generating the Zeeman splitting by using a parallel magnetic field [55, 56] and a significantly enhanced gap (the so-called minigap) that protects the end-localized MFs from thermal effects [61]. In addition, the nanowires can be arranged in networks that allow the manipulation of MFs for TQC [62, 63].

The 1D version of the semiconductor–superconductor heterostructure [54–56]—the so-called semiconductor Majorana nanowire—is a realization of the 1D topological superconductor (TS) model first proposed by Kitaev [23] in the context of TQC. In the presence of a small Zeeman splitting $\Gamma$, the Majorana nanowire with proximity-induced s-wave superconductivity is in a conventional superconducting state with no MFs, while for $\Gamma$ larger than a critical value $\Gamma_c$, localized MFs exist at the ends of the quantum wire. We emphasize that, in the proposals for the realization of Majorana fermions using semiconductor–superconductor hybrid structures, the Zeeman splitting plays the key role of lifting the degeneracy associated with the fermion doubling problem [64, 65]. In practice, the required Zeeman splitting can be obtained either by applying an external magnetic field, or by proximity to a ferromagnetic insulator. We note that the realization of Majorana fermions in a 3D topological insulator–superconductor heterostructure does not require a Zeeman field, since the fermion doubling problem is avoided by the spatial separation between the surface states localized on opposite surfaces. Furthermore, the Zeeman splitting does not represent the only solution to the fermion doubling problem [65]. For example, in the case of a topological insulator nanowire proximity-coupled to a superconductor [32, 66] the cure of the fermion doubling problem is ensured by the orbital effect of a magnetic field applied along the wire, while the corresponding Zeeman splitting is negligible. More generally, each proposal for realizing MFs in solid state systems has to contain a specific solution to the fermion doubling problem. Finally, we note that the MFs emerging in a Majorana nanowire can be detected by measuring the zero-bias conductance peak (ZBCP) associated with tunneling into the end of the wire [67, 68, 54, 69–71], or by detecting the predicted characteristic fractional AC Josephson effect [23, 72, 28, 55, 56, 73]. While these techniques have already been implemented experimentally, measurements involving the direct observation of non-Abelian Majorana interference will ultimately be required to validate the existence of the zero-energy Majorana bound states. In the past year, the semiconductor Majorana wire, which is the focus of this review, has attracted considerable attention as a result of the recently reported experimental evidence for both the ZBCP [74–78] and the fractional AC Josephson effect in the form of doubled Shapiro steps [79].
2. Theoretical background

2.1. Spinless \((p_x + ip_y)\) superconductor/superfluid

The spinless \((p_x + ip_y)\) superconductor (superfluid) is the canonical system that supports zero-energy MFs localized at the defects of the order parameter, such as vortices and sample edges [11]. In 2D, the mean-field Hamiltonian for such a system is given by

\[
H_{2D} = \sum_p \xi_p c_p^\dagger c_p + \Delta_0 \sum_p [(p_x + ip_y) c_p^\dagger c_{-p} + \text{h.c.}],
\]

where \(\xi_p = p^2/2m - \epsilon_F\), with \(\epsilon_F\) the Fermi energy, and spin indices are omitted because the system is considered spinless (or spin-polarized). The lowest energy solution of the BdG equations \(H_{2D} \Psi(r) = E \Psi(r)\) near a vortex or near the sample edges (where the order parameter \(\Delta_0\) vanishes), calculated under appropriate conditions, is non-degenerate and has zero energy \((E = 0)\), while the corresponding second quantized operator (the creation operator for the Bogoliubov state) is Hermitian, \(\gamma^\dagger \gamma = \gamma\). In 1D the zero-energy MF solutions occur near the ends of the wire and, as argued by Kitaev [23], should be observable in a fractional AC Josephson effect-type experiment. Although a spinless p-wave superconductor does not exist in nature, this example makes it clear that the three main ingredients that are important for realizing zero-energy MFs in a condensed matter system are superconductivity, chirality (i.e., the \(p_x + ip_y\) orbital form of the order parameter), and the spinless or spin-polarized nature of the system (which ensures that the zero-energy solution localized at a defect of the order parameter is non-degenerate).

Despite the possibilities opened by superconducting strontium ruthenate [80] and cold fermion systems with p-wave Feshbach resonance [47–50] of realizing the physical conditions necessary for the emergence of MFs, actually realizing and observing the MFs in these systems are challenging tasks. In strontium ruthenate, even if the required half-quantum vortices can be realized, the minigap \(\sim \Delta^2/\epsilon_F \sim 0.1\) mK (with \(\epsilon_F\) the Fermi energy and \(\Delta\) the magnitude of the p-wave superconducting order parameter) that separates the zero-energy MF bound states from the higher energy regular BdG excitations also localized at the vortex cores is unrealistically small. On the other hand, in cold fermion systems with p-wave Feshbach resonance in the unitary limit, even if the minigap \(\sim \Delta^2/\epsilon_F \sim \epsilon_F\) can be relatively large, the short lifetimes of the p-wave pairs and molecules represent a major experimental challenge.

The first major attempt to reproduce the essential physics of spinless p-wave superconductors using only s-wave pairing was made in [27], by using a heterostructure consisting of a 3D strong topological insulator and an s-wave superconductor. In the cold fermion context [51], it was shown that (also see [52]) an artificial, laser-induced, Rashba spin–orbit coupling and a Zeeman field, in conjunction with s-wave pairing interactions, can reproduce the topological superfluidity and MFs of spinless chiral p-wave superfluids using an s-wave Feshbach resonance. Later, the same approach that was used in the cold fermion context was applied to a solid state heterostructure where the spin–orbit coupling, Zeeman field, and s-wave superconductivity are provided by a semiconductor, a magnetic field or proximity to a magnetic insulator, and proximity to an s-wave superconductor, respectively. The proposed setups are shown in figure 1. As discussed below, in the semiconductor–superconductor heterostructure the two main ingredients (in addition to superconductivity) that are essential for realizing MFs, i.e., chirality and spinlessness, are provided by a Rashba-type spin–orbit coupling and by restricting the low-energy physics of the semiconductor to a single relevant Fermi surface (or an odd number of such surfaces).

2.2. Semiconductor–superconductor heterostructure

The Rashba SO-coupled semiconductor (e.g., InSb, InAs) with proximity-induced s-wave superconductivity and Zeeman splitting is mathematically described by the following
Bardeen–Cooper–Schrieffer (BCS)-type Hamiltonian:

\[ H = (\eta k^2 - \mu)\tau_z + \Gamma \hat{n} \cdot \sigma + \frac{\alpha}{2} (k \times \sigma) \cdot \hat{z} \tau_z + \Delta \tau_z, \]  

(3)

where \( \eta = 1/\hbar^* \), with \( \hbar^* \) being the effective mass of the charge-carriers, \( \mu \) is the chemical potential measured from the bottom of a pair of spin sub-bands (in this review by ‘band’, we always mean a pair of a spin-split sub-bands, the bands themselves being separated by the energy gaps due to lateral confinement), \( \alpha \) is the Rashba spin–orbit coupling constant, and \( \Delta \) is the s-wave superconducting pair-potential in the semiconductor, which is assumed to be proximity-induced from an adjacent superconductor. In addition, \( \hat{n} \) is a suitably chosen direction of the applied Zeeman spin splitting given by \( \Gamma = \frac{1}{2} g \mu_B B \), with \( g \) the effective Landé g-factor, \( B \) the applied magnetic field and \( \mu_B \) the Bohr magneton. Note that \( H \) is written in terms of the four-component Nambu spinor \((\eta_1(r), \eta_1(r), \nu_1(r), -\nu_1(r))\), and that the Pauli matrices \(\sigma_{x,y,z}, \tau_{x,y,z}\) act on the spin and particle–hole spaces, respectively. For a Zeeman splitting \( \Gamma \) larger than a critical value, \( \hat{n} \) describes a 2D topological superconductor when the direction of the Zeeman field is perpendicular to the plane containing the vector \( \mathbf{k} = (k_x, k_y) \), i.e., for \( \hat{n} = \hat{z} \). A 1D topological superconductor with \( \mathbf{k} = k_z \) is obtained for either \( \hat{n} = \hat{x} \) or \( \hat{n} = \hat{y} \). In general, a finite topological superconducting gap develops only if the component of the Zeeman field perpendicular to the effective \( k \)-dependent Rashba spin–orbit field is larger than a critical value.

The Hamiltonian in equation (3) has recently been studied extensively in the context of 2D, 1D and quasi-1D (multichannel) semiconductors [51–53, 81–83, 55, 56, 54, 84–87]. Two setups proposed for the experimental realization of this Hamiltonian physics described by this Hamiltonian are shown in figure 1. The system is characterized by a topological quantum critical point (TQCP) that corresponds to the critical Zeeman field \( \Gamma_c = \sqrt{\Delta^2 + \mu^2} \), where the quantity \( C_0 = (\Delta^2 + \mu^2 - \Gamma^2) \) changes sign. For \( C_0 > 0 \), the (low-\( \Gamma \)) state is an ordinary, non-topological superconductor that includes perturbative effects from the Zeeman field and the spin–orbit coupling but does not host MFs. However, for \( C_0 < 0 \), the (high-\( \Gamma \)) state has non-perturbative effects from \( \alpha \) and can support zero-energy MF states localized at the defects of the pair-potential \( \Delta \). Interestingly, the proximity-induced pair-potential \( \Delta \) itself remains non-zero and continuous across the TQCP [54, 88], and, consequently, the two superconducting states break exactly the same symmetries, namely the gauge and time-reversal symmetries. In the absence of topological defects and boundaries, the single-particle spectrum of the high-\( \Gamma \) phase is similar to that of the low-\( \Gamma \) phase, as both are completely gapped in the bulk. However, the high-\( \Gamma \) topological state can be distinguished from the non-topological superconductor at \( \Gamma < \Gamma_c \) by probing the topological defects and the boundaries, as they host MFs only for \( \Gamma > \Gamma_c \).

The topological quantum critical point \( \Gamma_c \) is marked by the vanishing of the single-particle minimum excitation gap \( E_0 \). By diagonalizing the Hamiltonian in equation (3) one obtains the lower branch of the quasiparticle excitation spectrum,

\[ E_k^2 = \Delta^2 + \bar{\varepsilon}^2 + r_k^2 - 2\sqrt{\Gamma^2 \Delta^2 + \bar{\varepsilon}^2 r_k^2}, \]

(4)

where \( \bar{\varepsilon} = \eta k^2 - \mu \) and \( r_k^2 = \Gamma^2 + \alpha^2 k^2 \). For \( \Gamma \) near \( \Gamma_c \), the minimum of \( E_k \) is at \( k = 0 \), which corresponds to the minimum quasiparticle gap \( E_0 \),

\[ E_0 = |\Gamma - \sqrt{\Delta^2 + \mu^2}|. \]

(5)

Note that \( E_0 \) vanishes exactly at \( C_0 = 0 \), marking the location of the TQCP as a function of \( \Gamma, \Delta, \) or \( \mu \). Furthermore, it has been shown that the quantity \( C_0 \) is the Pfaffian of the BdG Hamiltonian at \( k = 0 \), \( C_0 = Pf(H(k = 0)\sigma_\tau_0) \) [36]. The sign of \( C_0 \), which determines whether the system has 0 or 1 MFs, is related to the Pfaffian topological invariant \( Q \) (see equation (11)) given by the product of the Pfaffians of the BdG Hamiltonian at \( k = 0 \) and \( \pi \) [23]. Since the sign of the Pfaffian of the BdG Hamiltonian at \( k = \pi \) is generically positive, the sign of \( C_0 \) by itself determines whether the state of the semiconductor hosts 0 or 1 MFs (or, in general, an even or odd number of Majorana bound states). The topological invariant of the semiconductor–superconductor heterostructure is discussed in more detail in section 2.4.

2.3. Topological class

Recent work [89–91] has established that the quadratic Hamiltonians describing gapped topological insulators and superconductors can be classified into ten distinct topological classes that can be characterized by certain topological invariants. The 2D spinless chiral \((\rho_x, i\rho_y)\) superconductor in the weak-pairing phase (\( \mu > 0 \)) belongs to the topological class D, which is characterized by an integer \( Z \) topological invariant. This implies that, under appropriate conditions, the system can support \( Z \) number of chiral Majorana edge modes that remain protected against small perturbations. The analogous system of a 2D Rashba-coupled semiconductor with \( \Gamma > \Gamma_c \) is also characterized by a \( Z \) invariant and supports \( Z \) gapless chiral Majorana edge modes with dispersion \( E_{edge}(k) = (\Delta/k_B)k \). Since the 2D system is in class D, it does it automatically imply that the corresponding 1D or quasi-1D system is also in class D? The topological class of the 1D nanowire can be guessed from a heuristic dimensional reduction argument. The MF mode in a 1D wire (say, along the \( x \)-axis) can be viewed as the dimensionally-reduced version of the chiral Majorana edge mode of a 2D system on an edge parallel to the \( y \) axis. From the mathematical equivalence, \( H_{\text{BdG}}^{\text{2D}}(k_y = 0) = H_{\text{BdG}}^{\text{1D}} \), where \( H_{\text{BdG}}^{\text{2D}} \) is the BdG Hamiltonian near an end of the wire, and the property \( E_{\text{edge}}(0) = 0 \), it follows that the end of the wire supports a zero-energy eigenstate. Since in 2D there are \( Z \) allowed chiral edge modes, it follows that in 1D there must be, under appropriate conditions, \( Z \) zero-energy MFs. Thus, the nanowire should also be characterized by a \( Z \) (not \( Z_2 \)) invariant, and, consequently, the purely 1D Majorana nanowire should belong to the BDI topological class.
To reveal the appropriate BDI classification for the nanowire and the associated Z invariant, it is necessary to identify a hidden chirality symmetry of the 1D system [92, 61]. In 1D, the Hamiltonian in equation (3) anticommutes with a unitary operator $S = \tau_z$, where the chirality symmetry operator $S$ can be written as the product of an artificial ‘time reversal’ operator $K$ and a particle–hole transformation operator $\Lambda = \tau_x \cdot \tau_y \cdot K$. Here, $K$ is the complex conjugation operator. The existence of all three symmetries—‘time reversal’, particle–hole, and chirality—ensures that the Hamiltonian is in the BDI symmetry class [89–91] characterized by an integer topological invariant. Under invariance of this symmetry, the strictly 1D nanowire can support an arbitrary integer number $N (= \bar{Z})$ of protected zero-energy MFs at each end. The situation is similar to that of a 1D spinless $p$-wave superconductor, which was shown [93] to support any integer number of MFs at each end. However, for the semiconductor Majorana wire, the experimentally realistic case of a quasi-1D system retains only an approximate chirality symmetry (the chirality symmetry is weakly broken by the inter-band Rashba coupling, which no longer commutes with $S$ [61, 94]) and allows multiple near-zero-energy modes at each end for values of the Zeeman coupling close to the confinement energy gap and above. The existence of the near-zero-energy modes suppresses the gap protecting the MF end modes in certain parameter regimes characterized by $\Gamma$ larger than the confinement energy [61, 94]. Further consequences of the chirality symmetry for the electrical conductance are discussed in [95].

2.4. Topological invariant

The topological class and topological invariant of the semiconductor–superconductor heterostructure is analogous to that of a spinless $p_x + ip_y$ superconductor. For the topological invariant of the 2D spinless $p_x + ip_y$ superconductor (which is in class D), we rewrite the Hamiltonian in equation (2) in the particle–hole basis $(c_k^+, c_k^-)$ as

$$H_{2D}^p = \xi_k \tau_z + \Delta_x k_x \tau_x - \Delta_y k_y \tau_y, \quad (6)$$

where we have allowed for different pair potentials $\Delta_x, \Delta_y$ along the $x, y$ directions. Writing the Hamiltonian in terms of the Anderson pseudo-spin vector [96] $\hat{d}(k)$ as $H_{2D}^p(k) = \hat{d}(k) \cdot \tilde{\tau}$, one can observe that in $D = 2$ all three components of $\hat{d}$ are non-zero. The topological invariant is an integer, as $Z$ is the relevant homotopy group $\pi_2(S^2)$ of the mapping from the 2D $k$ space to the 2-sphere of the three-component unit vector $d = \hat{d}/|\hat{d}|$ [17, 11]. On the other hand, in $D = 1$, the corresponding BDI can be made purely real (e.g., $\Delta_y$ drops out from equation (6) if the system is along the $x$-axis) and the vector $\hat{d}$ has only two components. Now, since the $k$-space is also one-dimensional, the topological invariant must again be in $Z$ (class BDI) since $\pi_1(S^1) = Z$. This invariant is simply the winding number,

$$N = \frac{1}{2\pi} \int_0^{2\pi} \theta(k) \, d\theta(k), \quad (7)$$

where $\theta(k)$ is the angle the unit vector $\hat{d}$ makes with, say, the $z$-axis in the $x$–$z$ plane. The winding number counts the number of times the two-component vector $\hat{d}$ makes a complete circle as $k$ varies in the 1D Brillouin zone.

The topological invariant for the semiconductor–superconductor heterostructure can be defined in a similar way to the spinless chiral $p$-wave superconductor. One needs, however, to account for the higher dimensionality of the Hamiltonian matrix in equation (3) and the consequent generalization of the winding number invariant. It is clear that in $D = 2$ the Hamiltonian in equation (3) cannot be made real because of the complex Rashba term. In contrast, in $D = 1$, $H$ can be made purely real, but the components of the $\hat{d}$-vector in the $4 \times 4$ Hamiltonian are themselves $2 \times 2$ matrices. More generally, the BdG Hamiltonian of a TS system in $D = 1$, despite being real (thus preserving the chiral symmetry given by the operator $S = \tau_z$), can be a large $2N \times 2N$ square matrix. Using the general framework for chiral symmetric systems [97, 98], the integer topological invariant for this system can still be defined [92, 61] by generalizing the concept of the $\hat{d}$-vector winding number for arbitrary dimensionless matrices. Since, as discussed in section 2.3, $H$ anticommutes with the chirality operator $S = K \cdot \Lambda = \tau_x \cdot \tau_y$, $H$ can be expressed as a block off-diagonal matrix in a basis that diagonalizes the unitary operator $S$:

$$U \tilde{H}(k) U^\dagger = \begin{pmatrix} 0 & A(k) \\ A^T(-k) & 0 \end{pmatrix}. \quad (8)$$

Following [92, 61] one can now define the variable,

$$z(k) = \exp(i \theta(k)) = \text{Det}(A(k))/|\text{Det}(A(k))|, \quad (9)$$

and calculate the topological invariant,

$$W = -\frac{i}{\pi} \int_{k=0}^{k=\pi} \frac{dz(k)}{z(k)}, \quad (10)$$

which is an integer, including zero ($W \in Z$).

If the chirality symmetry is broken (it is weakly broken for quasi-1D multiband wires with transverse Rashba coupling $\alpha_y \neq 0$), the number of exact zero-energy MFs at each end of the wire goes back to 0 or 1. The corresponding $Z_2$ topological invariant is

$$Q = \text{sgn} \left\{ P[f(H(k = 0)\sigma_y \tau_y \times P[f(H(k = \pi)\sigma_y \tau_y)] \right\}, \quad (11)$$

and the topological class for the quasi-1D system reduces from BDI to D. $Q = +1 (-1)$ represents the topologically trivial (nontrivial) state with 0 (1) MF at each end of the wire. In the presence of the chirality invariance in 1D, it can be shown that $Q$ gives the parity of the integer topological invariant $W$, in analogy to the 2D case where $Q$ for the semiconductor–superconductor heterostructure gives the parity [36] of the first Chern number topological invariant, which is an integer.

2.5. Minigap

The minigap for topological superconductors is defined as the energy of the first excited regular fermion state
(above the zero-energy MF state) in either the bulk or the edge of the system. This gap is responsible for the thermal protection of the MFs and, consequently, for the nontrivial physics associated with them, such as non-Abelian statistics, by protecting the Majorana bound state from mixing with regular fermion states above the minigap. In naturally occurring quasi-2D chiral-p wave superconductors, such as strontium ruthenate, even if the MFs are realized in the cores of the half-quantum vortices, the minigap $\Delta \sim \Delta^2/\epsilon_F \sim 0.1 \text{ mK}$ is unrealistically small. In chiral p-wave superfluids, potentially realizable using cold fermions with p-wave Feshbach resonance, this is less of a problem, because in this case $\Delta \sim \epsilon_F$ and the minigap $\Delta^2/\epsilon_F$ is of order $\Delta$. In solid state hybrid structures, the minigap has to be large enough so that the experiments can access the MF physics at realistically achievable temperatures. This is one important experimental aspect in which the semiconductor nanowire heterostructure has a significant advantage over the corresponding 2D systems. In the 1D system, the minigap naturally scales with the induced superconducting gap (see equation (5)), while this is generically not the case for the 2D systems (see, however, [81]).

The reason why the minigap in the nanowires is greatly enhanced over the 2D heterostructures can be understood from the dimensional reduction arguments. In going from the 2D plane to the 1D wire, as the width the dimensional reduction arguments. In going from the 2D enhanced over the 2D heterostructures can be understood from the physics at realistically achievable temperatures. This is one important experimental aspect in which the semiconductor nanowire heterostructure has a significant advantage over the corresponding 2D systems. In the 1D system, the minigap naturally scales with the induced superconducting gap (see equation (5)), while this is generically not the case for the 2D systems (see, however, [81]).

2.6. Phase diagram of semiconductor Majorana wire, sweet spots, and approximate chirality symmetry

In a strictly 1D wire with proximity-induced superconductivity the Majorana-supporting topological phase emerges at Zeeman fields higher than the critical value [54, 52]

$$\Gamma_c = \sqrt{\Delta^2 + \mu^2}. \quad (12)$$

Consequently, for $\Gamma < \Gamma_c$ the superconducting phase is topologically trivial, while for $\Gamma > \Gamma_c$ the topological phase is realized. How is this simple picture modified in a quasi-1D system with multiple occupied confinement bands? If the applied Zeeman field is much smaller than the spacings between the confinement bands, nothing much is changed, except that $\mu$ in equation (12) has to be understood as the chemical potential measured from the bottom of the topmost occupied band (also called the Majorana band). However, the phase diagram is nontrivially modified when the Zeeman field is comparable to or higher than the spacings between the confinement bands.

Consider a finite-width wire oriented along the $x$ direction and proximity-coupled to an $s$-wave superconductor, with the interface perpendicular to the $z$ direction. The effective spin–orbit field generated by Rashba coupling is oriented along the $y$ direction. Two phase diagrams of this quasi-1D Majorana wire are shown in figures 2 and 3. The main difference between the two diagrams is due to the different orientations of the Zeeman field: in figure 2 the field is perpendicular to the semiconductor–superconductor interface, while in figure 3 it is oriented along the wire. In both cases the Zeeman field is perpendicular to the effective spin–orbit field generated by the Rashba coupling. Note that, when the magnetic field is parallel to the $z$ axis, the normal state spectrum is characterized by anti-crossings of the sub-bands corresponding to transverse $n_x$ modes with opposite parity (see figure 2, red circles). By contrast, when the magnetic field is parallel to the wire, these bands cross at the 'sweet spots' [85], critical points where (in the absence of inter-band pairing) two topologically trivial and two topologically nontrivial phases meet. We emphasize that inter-band pairing stabilizes the topological phase in the vicinity of the sweet spots (see figure 3; more details about sweet spot physics are provided in appendix A). By contrast, rotating the field away from the $x$ direction favors the topologically trivial superconductor (SC) phase.

The phase diagram in figure 3 reveals that, upon increasing the Zeeman field, the system undergoes a series...
of topological quantum phase transitions as it traverses successive topologically trivial and nontrivial phases. These phases are characterized by a certain number $N$ of low-energy modes localized at each end of the wire. In the thin wire limit, $L_y \to 0$, these modes become zero-energy Majorana bound states. In a finite-width wire, for $N$ even, the low-energy modes acquire a small non-zero gap, while for $N$ odd, $N - 1$ modes become gapped and one mode (the Majorana mode) remains gapless. The opening of the small low-energy gap is due to the inter-band Rashba coupling [94, 61], (see, for example, the inter-band Rashba term given by equation (B.4) in appendix B), that breaks the hidden chirality symmetry of the purely 1D model [92, 61].

Finally, we note that in the limit of weak semiconductor–superconductor (SM–SC) coupling, the location of the phase boundaries is closely related to the non-superconducting SM spectrum [99]. However, the locations of the phase boundaries (in particular the boundary between the $N = 0$ and 1 phases) depends strongly on the coupling strength [86]. Specifically, from equation (12) the minimal Zeeman field necessary for reaching the topological phase in the single-band case is $\Gamma_{c0} = \Delta$. This critical field corresponds to the transition between the $N = 0$ and 1 phases at low values of the chemical potential. For a multiband system, we have to take into account the band dependence of the induced gap $\Delta_{n'}$ and the proximity-induced energy renormalization $\Gamma_{ren}$ (see section 3.3 for details). Within the decoupled band static approximation (valid when the effective SM–SC coupling is much weaker than the inter-band spacing and the SC bulk gap), we find that the critical Zeeman field required for entering the topological phase with $N = 1$ is characterized by multiple minima $\Gamma_{c0} = \gamma_{nn}$ corresponding to values of the chemical potential at the bottom of each band $n$. Here, $\gamma_{nn}$ is the effective SM–SC coupling corresponding to band $n$. Consequently, increasing the coupling strength will move that phase boundary toward higher Zeeman fields. In addition, the presence of proximity-induced inter-band pairing widens the topological phase near the sweet spots and further reduces the dependence of $\Gamma_{c}$ on $\mu$ [86]. Experimentally, this may result in an apparent insensitivity of the critical magnetic field associated with the emergence of the Majorana bound state on the chemical potential. In addition, the inter-band pairing arising from a nonuniform coupling with the bulk superconductor results in a phase diagram characterized by a non-simply connected structure [86], which allows topological adiabatic pumping [100].

**2.7. Probing Majorana fermions I: zero-bias conductance peak and fractional AC Josephson effect**

The simplest way to establish the possible presence of a Majorana bound state at the end of a spin–orbit-coupled semiconductor wire with proximity-induced superconductivity is by performing a tunneling spectroscopy measurement. Since the MF state is a zero-energy bound state localized at the end of the wire, it is expected to produce a zero-bias conductance peak in the tunneling conductance $dI/dV$, similar to other zero-energy boundary states in superconductors [101, 102]. Here, $I$ is the current from the lead to the Majorana wire and $V$ is the applied voltage difference. The zero-bias conductance peak associated with tunneling into MFs is a result of resonant local Andreev reflection of the lead electrons at the lead–nanowire interface [69]. In a local Andreev process, the MF localized at the other end of the wire plays no role, provided the wire is long enough so that the two MF wavefunctions do not overlap. If there is a significant overlap between the MF wavefunctions, two other processes can also contribute to the transport current. One process corresponds to the direct transport of electrons via the conventional (Dirac) fermion state formed by the two overlapping MFs [103, 104, 68]. The second process is the crossed Andreev reflection, in which an incident electron from a lead coupled to one end of the wire is followed by a hole ejected into the lead coupled to the other end [105]. These two processes contribute to the non-local conductance or transconductance through the Majorana wire that we discuss in section 2.8. We note that the local Andreev reflection process typically gives rise to a non-zero sub-gap conductance even in the absence of MFs at the wire ends [106]. To suppress this background conductance, a gate-induced barrier potential may be applied at the lead–nanowire interface.

The presence of a zero-bias conductance peak represents a necessary, but not sufficient, condition for the existence of MFs that was theoretically proposed [67, 68, 54, 69–71, 86, 107–109] (see figure 4) and experimentally observed in recent measurements on quasi-1D semiconductor–superconductor hybrid structures [74–76]. The main problem concerning the unambiguous identification of such a zero-bias peak with...
end-localized MFs is that other sources of zero- or low-energy states localized at the wire boundary [110, 111] may produce similar zero-bias peaks. A more conclusive signature of MFs in a charge transport measurement is the quantized value of the $T = 0$ zero-bias conductance $I_c$ [69]. This value should be $2e^2/h$ for tunneling into a non-degenerate MF at the wire end, zero for the wire in the topologically trivial phase with no low-energy end state, and $4e^2/h$ in the presence of a conventional (non-Majorana) zero-energy state at the wire end. Such a conductance quantization, which can be taken as a smoking gun signature of MFs in semiconductor Majorana wires, has not yet been observed and may be difficult to obtain under realistic experimental conditions [112, 113].

Another proposal for detecting the existence of MFs in semiconductor wires involves the Josephson effect. In a Josephson junction (JJ) between two topologically trivial s-wave superconductors maintained at a phase difference $\phi$, the Josephson supercurrent $I$ is related to $\phi$ as $I = I_c \sin \phi$, where $I_c$ is the Josephson critical current. In a Josephson junction between topological superconducting wires with end state MFs, this relation changes to $I = I_c \sin \phi/2$ [23, 72, 28]. Consequently, if the phase difference $\phi$ is controlled by a magnetic flux threaded through a loop containing the Josephson junction, the periodicity of the Josephson current changes from $2\pi$ to $4\pi$ as the semiconductor Majorana wire is tuned through the TQPT [55, 56]. In practice, the doubling of the period of the Josephson effect can be measured by applying a small voltage $V$ across the junction and measuring the AC Josephson effect. The frequency of the AC Josephson effect in the TS phase, $eV/h$, is half the conventional Josephson frequency, $2eV/h$, obtained in the topologically trivial superconducting phase. Note that the use of the AC Josephson effect is necessary to avoid the inelastic relaxation between the two branches of the local Andreev bound states involved in the Josephson effect [72].

There are several ways to understand the change in the periodicity of the AC Josephson effect in the presence of MFs. Mathematically, it can be understood as a change in the dependence of the energies of the Andreev bound states at the junction on the phase difference $\phi$. While in the absence of the MFs the energy of the Andreev bound state goes as $E \propto \cos \phi$, with MFs this formula changes to $E \propto \cos \phi/2$. Since the Josephson supercurrent $I$ is related to the Andreev bound state energy as $I = (2e/h) dE/d\phi$, it follows that the period of the supercurrent, $I \propto \sin \phi/2$, is doubled in the presence of the MFs. In order for this period doubling to be observable, it is necessary for the two branches of the Andreev bound states, $\pm E$, to maintain their occupation number as $\phi$ is varied adiabatically. For DC Josephson effect this is impossible at thermodynamic equilibrium due to quasiparticle poisoning effect (the higher (lower) energy state is unoccupied (occupied)) [72]. In the AC Josephson effect, provided the period of the Josephson oscillations is shorter than the inelastic relaxation between the two branches $\pm E(\phi)$, the Josephson period doubling may be observable via the fractional frequency $eV/h$.

The doubling of the Josephson period in $\phi$ can also be understood from purely topological considerations. The fermion parity of the ground state of the topological superconductor (which is in the form of a ring with a weak link in the Josephson set up) flips as the threaded flux changes by $2\pi$. With a $2\pi$ flux change the superconductor is thus in an excited state with an electron from the ground state ejected to the junction and held between the two MF states. Only with a total flux change of $4\pi$ can the ground state fermion parity flip back and the electron leave the state formed by the MFs. This makes the junction return to the original state and consequently doubles the period of the Josephson effect from $2\pi$ to $4\pi$ [11, 23].

Even though the fractional Josephson effect is a robust signature of MFs, such an effect cannot be ruled out in ballistic S–N–S junctions and in JJs made of 1D p-wave superconducting wires such as the quasi-1D organic superconductors [72]. However, in fermion parity protected superconductors, the MF mediated fractional Josephson effect is topologically protected while there is no such robustness (for instance, to disorder in the ballistic S–N–S junctions, or to magnetic fields in p-wave wires) in the other two systems. Nevertheless, the fractional Josephson effect in semiconductor Majorana wires is susceptible to the quasiparticle poisoning effect [72], as well as to the non-adiabaticity effects [114].
The latter effect, in particular, shows that the fractional Josephson effect cannot be taken as an unambiguous signature of MFs because half or other fractional frequencies are in principle possible even in junctions between conventional superconductors. For recent work on the fractional Josephson effect in the limits of strong tunneling and long junctions, see [115, 116]. Experimental evidence of the fractional AC Josephson effect in the form of doubled Shapiro steps has been reported in semiconductor Majorana wires [79]. In this review we will not further discuss this effect, but will focus instead on experiments targeting the zero-bias conductance peak.

2.8. Probing Majorana fermions II: quantum non-locality, transconductance, and interference

Neither the non-quantized zero-bias conductance peak, nor the fractional AC Josephson effect, could constitute a sufficient proof for the existence of MFs in semiconductor–superconductor heterostructures, as in principle they can arise even in the absence of MFs. However, a conclusive experimental proof could be obtained by making use of the intrinsic non-local properties of these states. In MFs, non-locality stems from the absence of an occupation number associated with them individually. To define the electron occupation number in terms of spatially separated MFs, one must consider a pair of MFs, $\gamma_a$, $\gamma_b$, and define the second quantized electron creation operator as $d^\dagger = \gamma_a + i\gamma_b$. The quantum state of the system is then determined by the eigenvalues of the electron occupation number operator $n_d = d^\dagger d = 0, 1$. Since $n_d$ is related to the MF operators by

$$n_d = \frac{1 + i\gamma_a\gamma_b}{2},$$

it follows that the state of the whole system is determined by non-local correlations between the spatially separated MFs $\gamma_a$ and $\gamma_b$. An idea to probe this non-locality involves injecting an electron into one end of the Majorana wire and retrieving it at the opposite end. By connecting leads to the left and right ends of a wire that hosts MF states localized near the two ends, one could imagine that an electron injected into end $a$ flips the occupation number $n_d$ from $n_d = 0$ to $1$. The injected electron can then escape from end $b$, flipping the occupation number of the nanowire state back to $n_d = 0$. Such a process, where an electron can enter from one end and exit at the other end as an electron, can be viewed as Majorana-assisted electron transfer. As has been discussed before [103, 104, 68], such a transfer should not violate the locality and causality principles. In other words, in the absence of an overlap between the two MF wavefunctions, the probability of an electron appearing at end $b$ becomes completely independent of the lead-wire voltage difference applied at the opposite end [68]. Hence, there is no violation of causality. The non-local conductance (transconductance), given by $dI_b/dV_a$, can only be non-zero when there is a finite overlap between the two MF wavefunctions. However, in addition to the Majorana-assisted electron transfer, a second source [105] for non-zero transconductance is represented by the crossed Andreev reflection (CAR), also known as Cooper pair splitting. In this process an electron injection into a Majorana bound state at one end is followed by the emission of a hole from a second Majorana state at the other end. The net result is the injection of a Cooper pair in the topological superconductor nanowire. The CAR contribution to transconductance, which is opposite in sign to the contribution arising from Majorana-assisted electron transfer, is also non-zero only when the wavefunctions of the two MF states overlap [105]. It has been shown that [117], in the case of symmetric tunneling between the two leads and the MFs ($I_a = I_b = t$), the transconductance in the semiconductor Majorana wire is given by

$$\frac{dI_b}{dV_a} = \frac{32V_a}{16\Gamma^2 + (\delta^2 - V_a^2)^2 + 8\Gamma^2(\delta^2 + V_a^2)},$$

(14)

Here, $V_a$ is the voltage at end $a$, $I_b$ is the current at end $b$, $\Gamma \propto i\tau$ is the lead-induced broadening of the MF level, and $\delta$ is the overlap integral between the two MF wavefunctions. Note that the transconductance vanishes in the limit $\delta \rightarrow 0$, which is consistent with earlier results [104, 68, 105]. Even when the direct wavefunction overlap of the MFs is vanishingly small, an effective coupling between the MFs, and consequently a non-zero Majorana-assisted electron transfer amplitude, may be present if the topological superconductor has an appreciable charging energy [118]. In this case, both the Majorana-assisted electron transfer and CAR can result in a non-zero transconductance between the leads. Recently, the shot noise and the current–current correlations due to CAR have been proposed as possible experimental signatures of end state MFs [119].

Even the MF-induced transconductance, while interesting and nontrivial, cannot be considered as a definitive signature of MF modes because conventional near-zero-energy states (such as those produced by localized impurities) trapped near the contacts with the leads can also produce such non-local signatures in the presence of superconductivity [117]. On the other hand, a non-local tunneling spectroscopy interference experiment, similar to earlier interference-based proposals in topological insulators and superconductors [30, 29, 120, 118], has recently been suggested as capable of providing a direct verification of the non-local physics of 1D wires containing end MFs [117]. The effect requires non-local fermion parity [121], which is unique to topological systems and cannot be emulated by conventional near-zero-energy Andreev states or any other local excitations near the wire ends. The proposed scheme, where the tunneling amplitude is measured as a flux dependence of an energy level and the fermion parity is fixed by a superconducting single-electron transistor configuration, is suitable for unambiguous experimental testing of the presence of MFs in semiconductor Majorana wires. We note that other methods for detecting MFs have also been proposed [122–127, 46, 128].

3. Realistic modeling of semiconductor Majorana wires

The construction of the effective low-energy model for a Majorana hybrid structure involves three main steps:
developing a tight-binding model for the component that provides spin–orbit coupling (e.g., semiconductor, topological insulator, etc) and projecting onto a reduced low-energy subspace, (ii) incorporating the superconducting proximity effect, and (iii) defining an effective Hamiltonian based on a linear approximation for the frequency-dependent proximity-induced self-energy. Below, we provide the relevant details and point out the main approximations involved in this construction. In addition, we discuss several aspects of Majorana-supporting hybrid nanostructures that are not captured by simple models of ideal 1D systems, but represent critical components of the experimental realizations of Majorana nanowires, such as the presence of disorder and smooth confining potentials.

The system is characterized by a specific function for a given configuration of external gate potentials, the low-dimensional systems, as it generates a density-dependent interaction and will assume that

\[ H_{\text{tot}} = H_{\text{SM}} + H_{\text{int}} + H_{Z} + H_{V} + H_{\text{SC}} + H_{\text{SM-SC}}. \]  

where \( H_{\text{SM}} \) is a non-interacting model for the semiconductor component (or, in general, other spin–orbit-coupled material, e.g., topological insulator), \( H_{\text{int}} \) contains many-body electronic interactions, \( H_{Z} \) describes the applied Zeeman field, \( H_{V} \) contains terms that account for disorder and gate potentials, \( H_{\text{SC}} \) is the Hamiltonian for the superconductor, and \( H_{\text{SM-SC}} \) describes the semiconductor–superconductor coupling. Here, we will not address the problem of electron–electron interaction and will assume that \( H_{\text{int}} = 0 \). However, we emphasize that Coulomb interaction plays an important role in low-dimensional systems, as it generates a density-dependent renormalization of the electrostatic potential. Consequently, the Zeeman field \( \Gamma \) and the chemical potential \( \mu \) of a Majorana wire are not independent variables [129] and, for a given configuration of external gate potentials, the system is characterized by a specific function \( \mu = \mu(\Gamma) \). This has important experimentally observable consequences [129], as we will discuss in section 4. At the Hartree level, the effects of Coulomb interaction can be incorporated using a self-consistent scheme similar to that described in [130]. Below, we derive the low-energy effective model for the heterostructure described by equation (15) under the assumption \( H_{\text{int}} = 0 \).

### 3.1. Tight-binding models for semiconductor nanowires

The first element in the development of a low-energy effective theory for a Majorana-supporting hybrid structure is a tight-binding model for the spin–orbit-coupled component of the system (e.g., electron-doped SM, hole-doped SM, topological insulator, etc) corresponding to \( H_{\text{SM}} \) in equation (15). In general, when choosing the model, one has to strike a balance between accuracy and simplicity and one has to consider two key aspects: (i) the dimensional reduction from three dimensions (3D) to quasi-2D or quasi-1D, and (ii) the projection onto a reduced low-energy subspace. To illustrate some of the possible issues, we consider the case of electron-doped and hole-doped semiconductors.

The simplest tight-binding model for an electron-doped wire (or a thin film) is a two-band model with nearest-neighbor hopping. The natural starting point for constructing such a model is a 3D Hamiltonian for conduction electrons in the effective mass approximation,

\[ H_{0}(k) = \sum_{k,\sigma} \left( \frac{\hbar^{2}k^{2}}{2m^{*}} - \mu \right) c_{k\sigma}^\dagger c_{k\sigma}, \]  

where \( c_{k\sigma} \) is the annihilation operator for a particle with wavevector \( k \) and spin \( \sigma \), \( m^{*} \) the effective mass of the conduction band, and \( \mu \) is the chemical potential. In a thin film, the motion in the transverse direction is quantized and the transverse modes can be obtained by solving the quantum problem involving the single-particle Hamiltonian corresponding to equation (16) with the substitution \( k_{x} \to -i\delta_{x} \) and the confining potential \( V(z) \). In the presence of a transverse field that breaks inversion symmetry, the spin and orbital degrees of freedom are coupled and the effective Rashba-type spin–orbit interaction (SOI) is described by

\[ H_{\text{SOI}}(k) = \alpha_{R} \sum_{k,\sigma} \left( c_{k}^\dagger (k_{x}\sigma_{x} - k_{y}\sigma_{y}) c_{k} \right), \]  

where \( k = (k_{x}, k_{y}) \), \( \alpha_{R} \) is the Rashba coefficient, \( \sigma_{x} \) are Pauli matrices, we have used the spinor notation \( c_{k}^\dagger = (c_{k}^\dagger, c_{-k}^\dagger) \), and we have assumed that only one transverse mode is relevant to the low-energy physics. The physics described in the long-wavelength limit by the Hamiltonian \( H_{0} + H_{\text{SOI}} + H_{V} \), where \( H_{V} \) represents the contribution from the confining potential, can be also determined using a tight-binding model defined on a lattice. For example, considering a simple cubic lattice with constant \( a \) and nearest-neighbor hopping, the semiconductor Hamiltonian reads

\[ H_{\text{SM}} = H_{0} + H_{\text{SOI}} = -t_{0} \sum_{i,\delta} \left( c_{i+\delta\uparrow}^\dagger \sigma_{x} c_{i\uparrow} - c_{i+\delta\downarrow}^\dagger \sigma_{y} c_{i\downarrow} + \text{h.c.} \right) + \frac{i\alpha_{R}}{\sqrt{2}} \sum_{i,\delta} \left[ c_{i+\delta\uparrow}^\dagger \sigma_{y} \delta_{i} - c_{i+\delta\downarrow}^\dagger \sigma_{x} \delta_{i} + \text{h.c.} \right]. \]  

where \( H_{0} \) includes the first two terms and describes nearest-neighbor hopping on a simple cubic lattice and the last term represents the Rashba spin–orbit interaction. Here, \( i = (i_{x}, i_{y}, i_{z}) \) labels the lattice sites, \( \delta \in \{ \delta_{x}, \delta_{y}, \delta_{z} \} \) are nearest-neighbor position vectors. The confining potential involves the additional local term \( H_{V} = \sum_{i,\delta} V(i) c_{i\delta}^\dagger c_{i\delta} \).

The parameters of the tight-binding Hamiltonian (18) are determined by the condition that \( H_{\text{SM}} \) and \( H_{0} + H_{\text{SOI}} \) describe the same physics in the long-wavelength limit \( \mathbf{k} \to 0 \). Consequently, the hopping parameter in (18) is \( t_{0} = \hbar^{2}a^{-2}/2m^{*} \) and the Rashba coupling is \( \alpha = \alpha_{R}/a \).
For hole-doped SMs, an effective tight-binding Hamiltonian can be obtained using a similar approach and starting from the Luttinger 4-band model [131, 132], \( \hat{H}_0(k) = \sum_k c_k^\dagger [\hbar \alpha J_3(k) = \mu] c_k \), where \( c_k \) and \( c_k^\dagger \) are four-component spinors. The single-particle Luttinger Hamiltonian is

\[
\hat{h}_L(k) = \frac{-\hbar^2}{m_0} \left[ \frac{2\gamma_1 + 5\gamma_2}{4} k^2 \right] - \gamma_2 \sum_i k_i^2 J_i - \gamma_3 \sum_{i \neq j} k_j J_i J_j, \tag{19}
\]

where \( m_0 \) is the free electron mass, \( k = (k_x, k_y, k_z) \) is the wavevector, \( J = (J_x, J_y, J_z) \) is a set of \( 4 \times 4 \) matrices representing angular momenta \( 3/2, 1/2 \), and \( \gamma_1, \gamma_2, \gamma_3 \) are the Luttinger parameters. We assume that the dominant contribution to the valence band comes from p-like orbitals, \( |X|, |Y|, \text{and } |Z| \), and that in the presence of SOI the top valence band corresponds to the eigenstates of the total angular momentum \( J \) with \( j = 3/2 \).

\[
\Phi_{\pm \frac{1}{2}} = \frac{1}{\sqrt{6}} \left[ \alpha \left( \pm |X| - i |Y| \right) \chi_{\pm} + \sqrt{\frac{2}{3}} |Z| \chi_{\pm} \right], \\
\Phi_{\pm \frac{3}{2}} = \frac{1}{\sqrt{2}} \left( \alpha |X| - i |Y| \right) \chi_{\pm}, \tag{20}
\]

where \( m = \pm 1/2, \pm 3/2 \) are the eigenvalues of \( J_z \) and \( \chi_{\pm} \) are spin eigenstates with \( S_z = \pm 1/2 \). The effective tight-binding model is constructed using the eigenstates (20) as a basis. More specifically, we consider an fcc lattice and nearest-neighbor hopping between the states \( \Phi_m(i) \) and \( \Phi_{m'}(j) \), where \( i \) and \( j \) are nearest-neighbor sites, with hopping matrix element \( t_{ij}^{mm'} \). The tight-binding Hamiltonian has the form

\[
H_0 = \sum_{m,m'} \sum_{i,j} t_{ij}^{mm'} c_m^\dagger c_{m'} - \mu \sum_{i,m} c_m^\dagger c_m, \tag{21}
\]

where \( c_m^\dagger \) is the creation operator for the state \( \Phi_m(i) \). If we consider the xy plane perpendicular to the (0, 0, 1) crystal axis, each site has four in-plane and eight out-of-plane nearest-neighbors. The corresponding hopping matrix elements can be expressed in terms of three independent parameters, \( t_1, t_2, \) and \( t_3 \). For example, the in-plane diagonal components are \( t_{\pm 3/2 \pm 3/2} = t_1 + 2t_2 \) and \( t_{\pm 1/2 \pm 1/2} = t_1 - 2t_2 \), while the diagonal out-of-plane hoppings can be written as \( t_{\pm 3/2 \pm 3/2} = t_1 - t_2, \) and \( t_{\pm 1/2 \pm 1/2} = t_1 + t_2 \). Finally, the values of the independent parameters are determined by the condition that the low-energy, long-wavelength spectrum of the lattice Hamiltonian (21) be identical to the spectrum of the Luttinger model. Explicitly, we have \( t_1 = \gamma \hbar J_3/m_0 a^2, \) \( i = 1, 3 \), where \( a \) is the lattice constant. For a hole-doped thin film with structural inversion asymmetry, the Rashba-type spin–orbit coupling is modeled phenomenologically by adding a term similar to \( H_{SOI} \) in equation (18), but for spin 3/2, i.e., with \( \sigma \to J. \) This SOI term induces a splitting of the top valence band (the heavy-hole band) that is proportional to \( k^3 \) in the limit \( k \to 0 \). This is in contrast to the linear splitting that characterizes the Rashba splitting of the conduction band modeled by the Hamiltonian \( H_{SM} \) from equation (18).

Note that, for both the 2-band model (18) and the 4-band Luttinger-type model, the effective Rashba coefficient \( \alpha \) is an independent parameter that does not depend on the confining potential \( V(i) \). Typically, in the numerical calculations \( V(i) \) is a hard-wall potential (zero inside a finite region and infinite otherwise) that does not break the structural inversion symmetry.

Expanding the basis (20) to include the eigenstates of the total angular momentum \( J \) with \( j = 1/2 \) (corresponding to the split-off band), as well as s-type states (corresponding to the conduction band), allows one to construct an 8-band tight-binding model for both electron-doped and hole-doped SMs that is equivalent in the long-wavelength limit to the 8-band Kane model [133]. There are two key differences between this model and the simpler models described above. First, the Rashba-type spin–orbit coupling in the 8-band model is determined implicitly by the asymmetric confining potential \( V(i) \) and does not involve any additional independent parameter. Consequently, this model captures the correlation between the strength of the spin–orbit coupling and the transverse profile of the wavefunction. In turn, this profile plays a key role in the SC proximity effect, as we will show in section 3.2. By contrast, these correlations are not captured by the simplified models. The second key difference becomes manifest when describing low-dimensional nanostructures. In the large length scale limit, the 2-band and 4-band models described above generate conduction and valence band spectra, respectively, that agree quantitatively with the results obtained using the 8-band model. This is illustrated in figure 5, which shows a comparison between the 3D spectra obtained using these models in the absence of spin–orbit coupling. The large discrepancies at wavevectors away from the \( \Gamma \) point suggest that for systems with reduced dimensionality these models will generate significantly different results. This behavior is illustrated in figure 6, which shows a comparison between the conduction band spectra of a SM film of thickness \( L_z = 50 \text{ nm} \) obtained using the 8-band and the 2-band models. In essence, the spectrum of the 8-band model is characterized by strong non-parabolicity and by a sub-band-dependent effective mass. Also, the quasi-2D effective mass predicted by the 8-band model is strongly dependent on the film thickness. These features cannot be reproduced by the simplified 2-band model. Moreover, similar discrepancies characterize the valence bands obtained using the 8-band and 4-band models. All these differences become even more apparent in quasi-1D nanostructures. Nonetheless, since Majorana physics is mainly controlled by a relatively small number of low-energy states, the simplified models can provide a reasonably accurate description of the semiconductor system with a proper choice of effective model parameters and within a limited range for the control parameters, i.e., chemical potential and Zeeman splitting.

An important aspect that has to be addressed when solving numerically a specific model for the Majorana wire is represented by the large number of degrees of freedom in the problem. We emphasize that Majorana fermions are zero-energy bound states localized near the ends of a SM...
wire that is proximity-coupled to a superconductor, hence we are interested in modeling a finite quasi-1D system with no particular symmetries, in the presence of disorder and external potentials. For a typical electron-doped SM nanowire modeled using the 2-band model (18) the number of degrees of freedom is of the order $10^7$–$10^8$. One possible solution is to use a coarse-grained lattice model with an effective lattice constant $a_{\text{eff}}$ much larger the actual SM lattice constant. For example, choosing $a_{\text{eff}} = 40a$ reduces the number of degrees of freedom to about $10^3$–$10^4$. However, while this is numerically convenient, it becomes difficult to address the short-range properties of the system, for example the effects of certain types of disorder. More importantly, the properties associated with Majorana physics are basically understood as resulting from the reduction of the quasiparticle degree of freedom to about $10^3$–$10^4$.

In addition, the simple models used in the calculations are expected to be highly inaccurate at high energy. The technical details associated with the projection onto a low-energy subspace are presented in appendix B for the case of the 2-band tight-binding model.

3.2. Proximity effect in semiconductor nanowire–superconductor hybrid structures

A critical ingredient of any recipe for realizing Majorana fermions in a solid state hybrid structure is the proximity-induced superconductivity. In essence, the electrons from the SM nanowire acquire SC correlations by partially penetrating in the nearby bulk s-wave superconductor. In conjunction with spin–orbit coupling, these correlations generate effective p-type-induced superconductivity in the SM nanowire. More specifically, each double degenerate confinement-induced band generates a combination of $p_x + i p_y$ and $p_x - i p_y$ superconductivity. Further, the Zeeman splitting breaks time-reversal symmetry and selects one of these two combinations, making the SM nanowire a direct physical realization of Kitaev’s toy model for a 1D spinless p-wave superconductor [23]. While induced pairing is the most prominent aspect of the proximity to the bulk superconductor, another effect is the renormalization of the energy scale for the nanowire. Qualitatively, this renormalization can be understood as resulting from the reduction of the quasiparticle weight of the low-energy SM states due to the partial penetration of the corresponding wavefunctions into the SC. As a consequence, the low-energy effective model for the nanowire will contain rescaled values of the original parameters (e.g., hopping parameters, spin–orbit couplings, Zeeman field, etc), as we show below in section 3.3.

To address quantitative aspects of the SC proximity effect, one has to consider specific models for the relevant terms in the total Hamiltonian (15): $H_{\text{SC}}$, which describes s-wave bulk superconductor, and $H_{\text{SM–SC}}$, representing the SM nanowire–superconductor coupling. At this point, one possible approach is to treat the pairing problem self-consistently [134–136] in order to account for spatial variations of the order parameter near the interface and effects due to interactions inside the nanowire [137–140] and the presence of a magnetic field. In this work, we will not discuss this aspect of the proximity effect and will model the bulk semiconductor at the mean-field level using a simple tight-binding Hamiltonian characterized by a constant pairing amplitude $\Delta_0$. Explicitly, we have

$$H_{\text{SC}} = \sum_{ij,\sigma} \left( \frac{\tilde{t}_{ij}}{\delta} - \mu_{\text{sc}} \delta_{ij} \right) \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \Delta_0 \sum_i \left( \hat{a}_{i\uparrow}^\dagger \mathbf{a}_{i\uparrow}^\dagger + \hat{a}_{i\downarrow} \mathbf{a}_{i\downarrow} \right),$$

where $i$ and $j$ label SC lattice sites, $\hat{a}_{i\sigma}^\dagger$ is the creation operator corresponding to a single-particle state with spin $\sigma$ localized near site $i$, and $\mu_{\text{sc}}$ is the chemical potential. Similarity, we can write the SM–SC coupling as

$$H_{\text{SM–SC}} = \sum_{i,\mu,\sigma} \sum_{\kappa,\delta} \sum_{m,\sigma} \left( \frac{\tilde{t}_{\kappa \delta}}{\delta} \mathbf{c}_{\kappa \mu}^\dagger \mathbf{c}_{\delta m} \mathbf{a}_{i\sigma} + \text{h.c.} \right),$$
where \( \mathbf{i}_0 = (i_x, i_y, i_z) \) and \( \mathbf{j}_0 = (j_x, j_y, j_z) \) label lattice sites near the interface in the SM and SC regions, respectively, \( m \) is the quantum number that labels the SM states (e.g., if the SM is described by a 2-band model \( m = \sigma \)), and \( \tilde{t}_{\text{in}} \) are coupling matrix elements between SM and SC local states. Since we are interested in the low-energy physics of the SM nanowire, it is convenient to integrate out the SC degrees of freedom and define an effective action for the wire. In the Green function formalism, this amounts to including a surface self-energy contribution in the SM Green function \([141, 54, 87]\). The basic structure of this self-energy contribution is illustrated by the local term

\[
\Sigma_{\text{nn}}(\omega) = -|\tilde{t}|^2 v_F \left[ \frac{\omega + \Delta_0 \sigma_y \tau_z}{\sqrt{\Delta_0^2 - \omega^2}} + \zeta \tau_z \right],
\]

where \( |\tilde{t}| \) represents a measure of the SM–SC coupling, \( v_F \) is the surface density of states of the SC metal at the Fermi energy, \( \sigma_y \) and \( \tau_z \) are Pauli matrices associated with the spin and Nambu spaces, respectively, and \( \zeta \) is a proximity-induced shift of the chemical potential. Note that (24) contains an anomalous term proportional to \( \tau_z \) that describes the proximity-induced pairing. Also, the diagonal term, which is linear in frequency in the limit \( \omega \to 0 \), is responsible for the reduced quasiparticle weight and the corresponding energy renormalization. Since the basic aspects have been addressed by several authors \([141, 81, 54, 87, 142–144]\), we focus here on two problems that are critical to understanding the proximity effect in real SM–SC hybrid structures: (i) the role of multiband physics, and (ii) the dependence on specific features of the SM–SC coupling matrix elements.

3.2.1. Proximity effect in multiband nanowires. The key feature that differentiates the multiband case from its single-band counterpart is the emergence of proximity-induced inter-band pairing. In addition, the proximity-induced renormalization of the SM energy scales has a matrix structure, rather than being described by an overall factor. To illustrate these features, we consider an electron-doped SM nanowire with rectangular cross section and dimensions \( L_x \gg L_y \sim L_z \) in contact with an s-wave SC. The nanowire is modeled using the 2-band model (18) written in the basis \( \psi_n(i) \), as described by equations (B.1)–(B.6), and the SM–SC coupling is given by equation (23). For simplicity, we assume lattice matching between the SM and the SC and nearest-neighbor hopping across the interface, \( \tilde{t}_{\text{nn}} = \tilde{t}(i_r) \delta(i_L - i_r), \) where \( d = (0, 0, d) \) is a nearest-neighbor position vector. The dependence of \( \bar{i} = \bar{i}(i_r) \) reflects the possibility of nonuniform SM–SC coupling across the nanowire, as in the recent experiments by Mourik et al \([74]\). After integrating out the SC degrees of freedom, the effective surface self-energy can be written in the spinor basis \( \psi_n = (\psi_i, \psi_{i+}, \psi_{i-}, \psi_{n+}) \) as

\[
\Sigma_{nn'} = \sum_{i_x, i_y, i_z, i_x', i_y', i_z'} \psi_n^{i_x, i_y, i_z}(i) G_{\text{SC}}(\omega, \mathbf{j}_0, \mathbf{j}_0') \tilde{t}(i_r) \psi_n^{i_x', i_y', i_z'}(i),
\]

where \( \mathbf{j}_0 = \mathbf{i}_0 + \mathbf{d} \) and \( \mathbf{j}_0' = \mathbf{i}_0' + \mathbf{d} \) and \( G_{\text{SC}} \) is a matrix, containing both normal and anomalous terms, that represents the Green function of the superconductor at the interface. We note that there are three sources of proximity-induced inter-band coupling in equation (25): (i) the position dependence of \( G_{\text{SC}} \), (ii) the nonvanishing coupling between states with arbitrary values of \( n_z \) and \( n_z' \), and (iii) the position dependence of \( \bar{i} \).

The first source has not yet been explored, but could have significant effects when the SC itself has small characteristic length scales. To account for these effects, the SC Green function has to be calculated explicitly by taking into account all relevant details, including the size and geometry of the system. On the other hand, assuming a large superconductor with a planar surface, the SC Green function becomes \( G_{\text{SC}} = G_{\text{SC}}(\omega, i_x - i_x', i_y - i_y', i_z - i_z') \) and can be expressed \([141, 87, 86]\) in terms of its Fourier transform \( G_{\text{SC}}(\omega, \mathbf{k}_r) \approx \frac{1}{v_F} \left( \frac{\omega^2 + \zeta^2}{\sqrt{\Delta_0^2 - \omega^2}} \right) \). In this case, since the dependence of \( G_{\text{SC}}(\omega, \mathbf{k}_r) \) on the in-plane wavevector \( \mathbf{k}_r \) is very weak \([141, 86, 9]\), the surface self-energy contribution is practically local and does not represent an additional source of inter-band coupling.

The second mechanism, which couples different confinement-induced \( n_z \) bands, is due to the presence of the interface and does require any in-plane spatial inhomogeneity. Qualitatively, this coupling can be understood in terms of virtual processes in which an electron occupying a state from the \( n_z \) band tunnels into the superconductor, then returns to the SM wire into a state from a different band, \( n_z' \). Assuming uniform hopping \( \bar{i} \) across the interface, the effective coupling due to such processes depends on the values of the wavefunction at the interface and can be expressed as \( \gamma_{n, n'} = v_F |\tilde{t}|^2 \phi_{n}(i_0) \phi_{n'}(i_0) \), where \( \phi_{n} \) is given by equation (B.1). We note that the effect of this inter-band coupling becomes negligible in the limit of strong confinement, when \( \gamma_{n, n'} \) is much smaller than the inter-band gap.

The third source of proximity-induced inter-band coupling is due to non-homogeneous interface hopping, \( \bar{i} = \bar{i}(i_r) \). This mechanism is discussed in detail in \([86]\). The effective SM–SC coupling of a SM nanowire with rectangular cross section and nonuniform interface tunneling can be written as

\[
\gamma_{nn'} = \delta_{n, n'} \sum_{i_x, i_y, i_z} \phi_{n}(i_0) \phi_{n'}(i_0) \sum_{i_x=1}^{N_x} \sum_{i_y=1}^{N_y} \sum_{i_z=1}^{N_z} \frac{1}{\left( i_x - i_x' \right)^2 + \left( i_y - i_y' \right)^2 + \left( i_z - i_z' \right)^2} \phi_{n}(i_{x}) \phi_{n'}(i_{y}).
\]

Neglecting the spatial dependence of the SC Green function at the interface, the proximity-induced effective self-energy becomes

\[
\Sigma_{nn'} = -\gamma_{nn'} \left[ \frac{\omega + \Delta_0 \sigma_y \tau_z}{\sqrt{\Delta_0^2 - \omega^2}} + \zeta \tau_z \right],
\]

where \( \gamma_{nn'} \) is given by equation (26) and \( \zeta \) is a constant that depends on the details of the SC band structure. Note that equation (27) is valid for frequencies inside the SC gap, \( |\omega| < \Delta_0 \). Also, we emphasize that the discussion leading to equation (27) was based on the 2-band tight-binding model.
for the SM wire, which is constructed using s-type localized orbitals as a basis, with spin being the only internal degree of freedom. In more complex models, the local states are labeled by a quantum number \( m \neq \sigma \), or by a set of quantum numbers. The hopping matrix elements across the interface, which parametrize the coupling Hamiltonian (23), depend explicitly on these quantum numbers and, in turn, the proximity-induced surface self-energy will depend on the details of this coupling. An example illustrating the proximity effect for hole-doped SM nanowires is given in appendix C.

3.3. Effective low-energy Bogoliubov–de Gennes Hamiltonian for the Majorana wire

In the presence of proximity-induced superconductivity, the low-energy physics of the SM nanowire is described by the Green function matrix \( G_{nn'}(\omega) \), which includes non-zero anomalous terms. Using the results of sections 3.1 and 3.2, one can write the inverse of the Green function matrix as

\[
G^{-1}_{nn'}(\omega) = \omega - H_{nn'} - \Sigma_{nn'}(\omega),
\]

where \( H_{nn'} \) is the effective low-energy Hamiltonian for the SM nanowire in the Nambu space and \( \Sigma_{nn'}(\omega) \) is the proximity-induced self-energy. For an electron-doped wire described using the 2-band tight-binding model, the self-energy is given by equation (27), while the low-energy Hamiltonian can be obtained by expanding equation (B.6) to include both particle and hole sectors. Explicitly, we have

\[
H_{nn'} = \left[ \epsilon_n + \Gamma_\sigma \tau_z \delta_{nn'} + i \alpha \delta_{nn'} \right],
\]

where the relevant quantities are the same as in equation (B.6), \( \tau_z \) is a Pauli matrix in the Nambu space, and the identity matrices in the spin and Nambu spaces, \( \sigma_0 \) and \( \tau_0 \), respectively, have been omitted for simplicity. The eigenvalues of the low-energy states can be obtained by solving the Bogoliubov–de Gennes (BdG) equation

\[
\det[G^{-1}(\omega)] = 0,
\]

where the frequency is restricted to values inside the bulk SC gap, \( |\omega| < \Delta_0 \), and the Green function is given by equations (28)–(29).

Solving equation (30) numerically can be rather demanding, but one can further simplify the problem by noticing that the relevant energy scale for Majorana physics (e.g., the induced pair-potential \( \Delta \)) is typically much smaller than the bulk SC gap \( \Delta_0 \). Consequently, one can focus on the low-frequency limit \( |\omega| \ll \Delta_0 \) and consider the self-energy within the static approximation \( \sqrt{\Delta_0^2 - \omega^2} \approx \Delta_0 \). In the static approximation, equation (28) becomes

\[
G^{-1}_{nn'}(\omega) = \omega Q_{nn'} - H_{nn'} + \gamma_{nn'} (\sigma_1 \tau_y + \xi/\Delta_0 \tau_z),
\]

where \( \gamma_{nn'} = \delta_{nn'} + \gamma_{nn'}/\Delta_0 \) accounts for the proximity-induced normalization of the SM energy scales. Since \( Q_{nn'} \) is a positive definite matrix, the BdG equation (30) can be rewritten in the static approximation as \( \det[\omega - H^{\text{eff}}] = 0 \), where \( H^{\text{eff}} \) is a frequency-independent quantity that can be viewed as an effective BdG Hamiltonian for the SM nanowire with proximity-induced superconductivity. Explicitly, the effective Hamiltonian has the form

\[
H^{\text{eff}}_{nn'} = Z_{nn'} H_{nn'} Z_{nn'} - \Delta_{nn'} \sigma_1 \tau_y - \delta \mu_{nn'} \tau_z.
\]

The first term in the right-hand side of equation (31) represents the SM Hamiltonian renormalized by the proximity effect. Note that, in general, this proximity-induced renormalization is described by a matrix, rather than an overall factor \( Z \) representing the reduced quasiparticle weight. The renormalization matrix is the solution of the equation

\[
Z_{nn'} (\delta_{nn'} + \gamma_{nn'}/\Delta_0) Z_{nn'} = \delta_{nn'},
\]

where \( \gamma_{nn'} \) is the effective SM–SC coupling matrix. In the single-band limit, this reduces to the induced SC gap-pair potential \( \Delta = \gamma \Delta_0/|\gamma + \Delta_0| \). Finally, the last term in (31) describes proximity-induced energy shifts and inter-band couplings that have only a rather limited quantitative relevance, \( \delta \mu_{nn'} = \xi \Delta_{nn'}/\Delta_0 \).

We emphasize here a key aspect of the proximity effect in multiband SM–SC hybrid structures: the proximity-induced inter-band coupling and the induced inter-band pairing. These effects depend on both the details of the SM–SC coupling at the interface and the dimensions of the nanosystem. More specifically, considering a SM wire with rectangular cross section \( L_x \times L_z \), the inter-band effects become critical whenever the gaps \( \Delta_{E_{nn'}} \) separating different confinement-induced bands \( n = (n_y, n_z) \) are comparable to the bulk SC gap \( \Delta_0 \). This situation occurs in wide wires and in the ‘sweet spot’ regime [85, 86], when two spin sub-band become degenerate at finite Zeeman field. By contrast, in the limit \( \Delta_{E_{nn'}} \gg \Delta_0 \) the inter-band effects are negligible and one can treat the proximity effect in the decoupled band approximation, i.e., \( \gamma_{nn'} \approx 0 \) if \( n \neq n' \). In this approximation, the matrices describing the proximity effect become diagonal, e.g., \( \gamma_{nn'} = \gamma_n \delta_{nn'} \), and we have \( \tilde{Z} = 1/\sqrt{1 + \gamma_n/\Delta_0} \) and \( \Delta_n = \gamma_n \Delta_0/(\gamma_n + \Delta_0) \). Also, we note that there is a key difference between the proximity-induced inter-band effects associated with confinement in the directions normal and parallel to the interface, respectively. Specifically, assuming \( n_z = n_z' \), i.e., strong confinement in the normal direction (so that the low-energy physics is controlled by a single \( n_z \) mode), and a weaker confinement in the \( y \)-direction, along with nonuniform SM–SC hopping \( \tilde{t}_{ny} \), results in an effective SM–SC coupling \( \gamma_{ny} = \gamma_{ny_1} \) that contains nonvanishing off-diagonal terms. However, for typical SM–SC couplings, \( \gamma_{ny_1} \) becomes negligible when the difference \( |n_y - n_y'| \) is large, as one can infer from equation (26), and only neighboring \( n_y \) bands are significantly coupled. Consequently, when constructing the effective Hamiltonian (31) it is enough to consider a reduced number of \( n_y \) bands to obtain an
an accurate description of the low-energy physics. This scenario was investigated in detail in [86]. On the other hand, when the confinement in the $z$-direction is weak, bands with arbitrary $n_z$ become coupled, as $\gamma_{n_z n'_z} \propto \phi_n(i_{k_F})\phi_{n'}(i_{k_F})$. In this case, it is critical to include the high-energy $n_z$ bands in the calculation, as they renormalize the low-energy physics via proximity-induced virtual processes. The role of the proximity-induced inter-band coupling is studied in detail in [145]. It is found that the proximity-induced gap is strongly suppressed in the intermediate and strong tunnel coupling regimes whenever the SM thickness exceeds a characteristic crossover value determined by the band parameters of the SM [145]. Furthermore, the strong coupling regime is characterized by a small induced gap that decreases weakly with the SM–SC coupling strength [145], in sharp contrast to expectations based on the decoupled band approximation, which predicts an induced gap of the order of the bulk SC gap $\Delta_0$. An example of a low-energy spectrum for a SM thin film-SC slab heterostructure with uniform coupling across a planar interface, illustrating the theoretical scheme described above, is presented in appendix D.

### 3.4. Low-energy physics in Majorana wires with disorder

There are several types of disorder that may play a role in the low-energy physics of semiconductor–superconductor hybrid structures [86]: impurities inside the bulk $s$-wave SC, disorder in the SM nanowire, and disorder induced by random SM–SC coupling. Below, we mention a few representative sources that could generate these types of disorder and briefly discuss some of their main features. As a general remark, we point out that the theoretical treatment of disorder in semiconductor Majorana wires can be done along two different directions: calculations of disorder-averaged quantities and calculations involving specific disorder realizations. However, the low-energy physics of the nanowire (on a scale of the order of the induced gap) is controlled by a small number of quantum states, typically less than 100 (see, for example, figures E.1 and E.2, upper panels, in appendix E), having most of their spectral weight inside the SM wire. When disorder is located in the nanowire or at the interface, the energies and the wavefunctions characterizing these states depend significantly on the specific disorder realization and the relevance of the disorder-averaged quantities is questionable. The reason for this dependence can be understood qualitatively by noticing that features of the disorder potential with length scales smaller than $1/k_F$, where $k_F$ is the Fermi wavevector of the Majorana band, are irrelevant, since they are averaged over by the low-energy SM states. Typically, $1/k_F$ is of the order $10^2$ nm, hence the effective disorder potential in a nanowire of length $L_z \sim 1 \mu$m is characterized by a small number of scattering centers and, consequently, the details of the disorder potential become relevant. Disorder-averaged quantities provide a good description of the low-energy physics (for example, the value of the induced SC gap) in long wires [144], but do not capture the specific properties of a given small segment of that wire, or those of a short wire of similar length.

Scattering off impurities inside a disordered bulk superconductor has a negligible effect on the topological SC phase of the nanowire [146, 147]. In essence, this behavior is due to the fact that the SM effective impurity scattering rate involves higher-order SM–SC tunneling processes and is suppressed by the destructive quantum interference of quasiparticle and quasi-hole trajectories [146]. Consequently, static disorder in the superconductor does not suppress the proximity-induced topological superconductivity in the semiconductor.

By contrast, disorder in the SM nanowire or at the SM–SC interface can strongly affect the stability of the topological SC phase. Some of the generic features of the low-energy states in the presence of disorder are illustrated in appendix E. Possible sources of disorder are the random variations of the width of the SM wire and, in general, surface roughness, and random potentials created by charged impurities located on or near the surface of the wire [86]. Another possible source of disorder is represented by the random coupling at the semiconductor–superconductor interface [86, 148]. We note that this random coupling has a twofold manifestation: a fluctuating induced pairing potential and a random proximity-induced renormalization of the SM Hamiltonian (see section 3.3). In general, the suppression of topological superconductivity by disorder represents a serious challenge to the experimental realization of MFs. A recent proposal for optimizing the stability of the topological phase against disorder involves replacing the semiconductor wire by a chain of quantum dots connected by $s$-wave superconductors [149]. In addition to the adverse effect on the stability of the topological SC phase, the presence of disorder impacts the low-energy physics of SM–SC hybrid structures in a number of other ways, some of them being investigated theoretically in several recent studies. For example, it was shown that the topological quantum phase transition is characterized by a quantized thermal conductance and electrical shot noise power that are independent of the degree of disorder [151]. The robustness of the topological phase against disorder was shown to depend non-monotonically on the Zeeman field applied to the wire [152]. The interplay between disorder and interaction in one-dimensional topological superconductors was addressed in [153]. Also, it was shown that in systems with disorder located at the end of the wire the weight of the characteristic Majorana-induced ZBCP in the differential tunneling conductance is strongly enhanced by mixing of sub-bands [154]. On the other hand, the presence of disorder can generate a ZBCP even when the superconducting wire is topologically trivial due to the proliferation of disorder-induced low-energy states [111, 155], or due to the weak antilocalization resulting from random quantum interference by disorder [156]. A similar ZBCP can occur in the topologically trivial phase as a result of fermionic end states with exponentially small energy that emerge if the confinement potential at the end of the wire is smooth [110]. In the light of the recent experiments on semiconductor nanowire–superconductor hybrid structures, ruling out the alternative mechanisms for the conductance peak represents a serious challenge.
4. Recent experiments and theoretical interpretations

In this section we briefly summarize several recent observations of experimental signatures consistent with the realization of Majorana bound states in semiconductor nanowire–superconductor structures. We also discuss a number of apparent discrepancies between the observed features and the theoretical predictions based on simple model calculations for the Majorana wire.

4.1. Experimental signatures of Majorana fermions in hybrid superconductor–semiconductor nanowire devices

The observation of a zero-bias conductance peak in local tunneling conductance measurements on semiconductor nanowires coupled to an s-wave superconductor has been recently reported in [74]. This observation, which is consistent with the theoretical predictions, may represent the first experimental evidence of Majorana fermions in a condensed matter system. Soon after, observations of similar ZBCPs were reported by two other groups [75, 76] and, recently, by two more groups [77, 78]. Since there are significant differences among the experimental setups, establishing conclusively that the ZBCPs observed in different systems are due to the same mechanism remains a critical open question.

Below, we briefly summarize the main results of [74]. We mention that a measurement of the fractional AC Josephson effect has also been reported in [79]. The observation suggests the presence of a Shapiro step twice as high as the value expected for conventional superconductor junctions [79], which would be consistent with the presence of MFs.

As discussed in the previous sections, an optimal hybrid system capable of hosting Majorana bound states and of measuring the expected ZBCP should possess certain characteristics, such as (i) a large SC gap, to protect the MF and to allow tuning of the Zeeman field in a wide range without destroying the superconducting phase, (ii) a long-enough wire length, to accommodate Majorana bound states at the wire ends without large overlap, (iii) low disorder, (iv) the ability to control the chemical potential, and (v) the ability to tunnel from a normal lead, while minimizing the perturbation on the topological SC state. The basic experimental setup for the measurements reported in [74] consists of a InSb nanowire in contact with a superconductor (NbTiN) and a metallic (Au) lead, as shown schematically in the top panel of figure 7. To measure the differential conductance \( \frac{dI}{dV} \), a bias voltage is applied between the normal lead and the superconductor (SC), and a tunnel barrier is created in the region between the metallic lead and the SC segment of the nanowire by applying a negative voltage to a narrow gate. The InSb nanowire is characterized by a high \( g \)-factor \( (g \approx 50) \), as well as a strong spin–orbit (SO) coupling (the Rashba parameter is \( \alpha \approx 0.2 \text{ eV Å} \)), making it a good candidate for the realization of MFs in the presence of proximity-induced superconductivity. The barrier potential suppresses the background conductance due to Andreev precesses and helps to reveal the ZBCP generated by the possible presence of MFs that could emerge for values of the magnetic field above a certain critical value. The dependence of the differential tunneling conductance on the bias voltage for different values of the magnetic field is shown in the bottom panel of figure 7. Note that a ZBCP emerges when the applied magnetic field exceeds about 100 mT. The ZBCP is robust to further increasing of the magnetic field until about 400 mT, above which the single peak seems to split into a two-peak structure. These observations are consistent with the MF interpretation of the tunneling conductance, as shown, for example, by the theoretical predictions illustrated in figure 4.

An important consistency check on the MF interpretation of the ZBCP is the requirement that the peak must disappear if the angle between the applied magnetic field and the direction of the effective spin–orbit field vanishes. The likely orientation of the spin–orbit field is along the direction perpendicular to the wire, in a plane that is roughly parallel to the nanowire–SC and nanowire–substrate interfaces. The angle dependence of the ZBCP was measured in [74] (see figure 8) and found to be consistent with the Majorana scenario, thus strengthening the identification of the observed ZBCP with the presence of a MF bound state at the normal lead–nanowire interface.

The main observations reported in [74], in particular the emergence of a ZBCP at finite magnetic field, have been subsequently confirmed by other groups [75, 76]. The similarities are rather surprising, considering that many of the relevant parameters that characterize the devices measured in these experiments are very different from those of [74]. For example, the experiments reported in [76] use InAs nanowires in proximity to superconducting Al (instead of
of magnitude weaker than the quantized value of $2e/h$. Furthermore, the observed ZBCP is more than an order of magnitude weaker than the quantized value of $2e/h$. Recently, the observed ZBCP is more than an order of magnitude weaker than the quantized value of $2e/h$. Additionally, the observed ZBCP is more than an order of magnitude weaker than the quantized value of $2e/h$. Moreover, the observed ZBCP is more than an order of magnitude weaker than the quantized value of $2e/h$. It is worth noting that the observed ZBCP is more than an order of magnitude weaker than the quantized value of $2e/h$.

**4.2. Suppression of the gap closing signature at the topological quantum phase transition**

While the observations [74] of a ZBCP in conductance measurements on semiconductor nanowires coupled to superconductors may represent the first experimental evidence of MFs, the absence of any signature associated with the closing of the superconducting gap (see figure 7) at the critical magnetic field associated with the topological quantum phase transition (TQPT) casts serious doubt on the MF interpretation of the ZBCP. The closing of the quasiparticle gap at the TQPT is a fundamental theoretical requirement. The question is whether or not this gap closure has a visible signature when the system is probed experimentally. Reference [160] has offered a possible explanation for the observed non-closure of the gap at the quantum phase transition between the trivial superconductor and the topological superconductor supporting the MFs in the end-of-wire tunneling experiments. By solving numerically an effective tight-binding model for multiband nanowires with realistic parameters, it has been shown [160] that, in the vicinity of the topological transition, the amplitude of the low-energy states at positions near the ends of the wire may be orders of magnitude smaller than the amplitudes of the localized MFs. Consequently, if the chemical potential of the system is located near the bottom of a confinement-induced semiconductor band, the contributions of these low-energy states to the end-of-wire local density of states (LDOS), and hence to the tunneling conductance, are essentially invisible (see figure 9, middle panel). This behavior results in an apparent non-closure of the gap, as reflected by these local quantities, even though the magnetic field approaches the critical value and the system is driven through a TQPT. By contrast, the closing of the gap mandated by the topological transition is clearly revealed by other quantities, such as the total density of states (DOS) (see figure 9, top panel) and the LDOS near the middle of the wire (figure 9, bottom panel). A definite prediction of [160] is that a tunneling measurement near the middle of the wire should clearly reveal the closing of the gap at the critical field $\Gamma_c$, but the zero-bias peak associated with the presence of Majorana bound states should be absent.

Correlated with an end-of-wire measurement characterized by
a zero-bias peak for \( \Gamma > \Gamma_c \), this would constitute a powerful argument for the presence of zero-energy Majorana bound states. In addition, the model calculations have shown that the non-closure of the gap, as revealed by the end-of-wire LDOS, is a non-universal phenomenon. For example, if a local measurement is performed in a regime characterized by a value of chemical potential that is not close to the bottom of a semiconductor band (i.e., \( \Delta \mu \gg \Delta \)), the closing of the gap should be visible. This regime is illustrated in figure 4. Finally, we note that the dominant feature in the end-of-wire LDOS (see figure 9, middle panel) is due to states associated with low-energy occupied bands that have significant amplitudes near the ends of the wire. In certain conditions (e.g., in the presence of disorder or in systems with smooth confinement) these states can have energies lower than the bulk quasiparticle gap and, consequently, can provide substantial contributions to the in-gap LDOS.

4.3. Discriminating between Majorana bound states and garden variety low-energy states

Despite their conceptual simplicity, the zero-bias conductance peak experiments do not constitute a sufficient proof for the existence of Majorana bound states in semiconductor–superconductor hybrid structures. In a recent theoretical work [110], it has been shown that a non-quantized near-zero-bias peak, such as that observed in the recent experiments [74–76], can arise even without end state MFs, provided the confinement potential at the wire end is smooth. A non-quantized near-zero-energy peak at the wire ends has also been shown to occur due to strong disorder effects [111], even when the nanowire is in the topologically trivial phase. In essence, these near-zero-bias peaks occur at finite values of the Zeeman field, due to the proliferation of low-energy states in the presence of disorder (see section 3.4), or in wires with smooth confinement (see section 4.4). To discriminate between the different possible mechanisms responsible for the zero-bias conductance occurring in a tunneling experiment, a diagnostic signature for the Majorana-induced ZBCP has been recently proposed [161]. It was shown that, for smooth confinement at the ends of the wire, the emergence of the near-ZBCPs is necessarily accompanied by a signature similar to the closing of a gap in the end-of-wire local density of states. This signature occurs even though there is no corresponding quantum phase transition, as the system stays in the topologically trivial phase, and traces the Zeeman field dependence of the near-zero-energy states. In the absence of such a gap closing signature, a ZBCP is unlikely to result from the soft confinement effect [110]. Similarly, when the ZBCP appears at the wire ends from disorder effects (but without MFs), the emergence of the zero conductance is preceded by a signature similar to the closing of the gap [111, 161]. So far, among all the scenarios that have been considered, the topological phase transition scenario involving the emergence of the MFs is the only one consistent with a ZBCP that occurs beyond a certain critical magnetic field together with the apparent non-closure of the quasiparticle gap before the emergence of the ZBCP. Since this is precisely what is observed in the experiments in [74], these theoretical results strengthen the identification of the observed ZBCP with topological Majorana bound states localized at the ends of the wire.

We note that the presence of low-energy sub-gap states in systems with disorder and smooth confinement may have another important consequence with dramatic experimentally observable implications: the existence of a soft superconducting gap, i.e., a SC gap characterized by a nonvanishing density of states and a V-shaped sub-gap tunneling conductance even at very low temperatures. This feature is manifestly present in the experimental data [74] (see, for example, figure 7) and represents one of the most important open issues in this field. There are several critical aspects that need to be clarified, such as the origin of the in-gap spectral weight, why these in-gap contributions occur as a smooth background, rather than sharply defined peaks in the LDOS, and whether or not a Majorana-induced ZBCP can be well defined in a system with a soft gap. Recently, disorder induced by interface fluctuations was identified [162] as the likely source of the in-gap states responsible for the soft gap. Another theoretical work [161] has shown that there are two key ingredients that may explain the emergence of the soft gap in weakly confined wires: (i) a finite potential

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**Figure 9.** Top: density of states (DOS) as a function of \( B \) for a wire with four partially occupied bands (seven spin sub-bands) and a chemical potential near the bottom of the fourth band (for \( B = 0 \)). At the TQPT characterized by \( B_c \approx 0.2 \) T the bulk gap closes. Middle: local density of states (LDOS) at the end of the wire as a function of magnetic field. The strong finite energy features have a weak dependence on \( B \). For \( B > B_c \), the Majorana peak is clearly visible. Note that there is no visible signature of the bulk gap closing at the TQPT. Bottom: LDOS at the middle of the wire. Note the closure of the gap at the TQPT and the absence of the zero-energy Majorana peak. Figure adapted from [160].
barrier allows states with large spectral weight near the end to hybridize with metallic states from the leads, and (ii) states from lower energy bands can penetrate through the barrier, hybridize strongly with the metallic states, and generate a broad contribution to the LDOS. By contrast, the Majorana mode, which is associated with the top occupied band, couples weakly to the lead—hence it is weakly broadened and still generates a well-defined ZBCP on top of the smooth background.

4.4. Majorana physics in finite-size wires: a ‘smoking gun’ for the existence of the Majorana mode

It has recently been proposed [129] that direct observation of the splitting of the zero-bias conductance peak could serve as ‘smoking gun’ evidence for the existence of the Majorana mode. In essence, the Majorana bound states come always in pairs [23] that are localized near the ends of the wire, if the system is clean enough. In any finite wire, the wavefunctions of the two Majoranas overlap, leading to a splitting [163, 164, 112, 157] of the Majorana mode, which is a pure zero-energy mode only in the infinite wire limit. At fixed chemical potential, this hybridization-induced energy splitting is characterized by an oscillatory behavior that depends on the Fermi wavevector of the top occupied band and the length of the wire. By contrast, when the particle density is constant, the oscillations can be suppressed [129], but the splitting of the Majorana mode is still a generic feature. Furthermore, regardless of conditions, two independent tunneling measurements at the opposite ends of a wire should observe exactly the same splitting of the ZBCP [129], as long as: (i) the peak is due to Majorana splitting, and (ii) a single pair of Majorana bound states exists in the system. We emphasize that features other than the splitting itself observed in local measurements at the two ends of the wire may be completely different. If confirmed experimentally, this would constitute strong evidence for the existence of the elusive Majorana mode in semiconductor–superconductor structures.

In the presence of disorder, several states with energies lower than the induced SC gap will emerge (see section 3.4). The energies of these sub-gap states depend on the strength of the disorder and the values of the Zeeman field. However, the Majorana mode is still protected, as long as the disorder strength does not exceed a certain critical value, and, consequently, the hallmark signature described above should still be observable. Nonetheless, strong disorder can effectively cut the nanowire into two or more segments, which can each host a pair of Majorana bound states. A natural question concerns the fate of the splitting oscillations generated by these multiple Majorana bound states that emerge in the presence of strong scattering centers. To address this question, we consider a wire with rectangular cross section \( L_x \times L_z = 100 \times 40 \) nm, four partially occupied bands, and smooth confinement in the presence of a strong scattering center consisting of a potential barrier of height \( \Delta V \) located at distances \( L_{x1} \approx 0.6 \) \( \mu \)m and \( L_{x2} \approx 1.2 \) \( \mu \)m from the two ends of the wire, respectively. The confinement and the barrier are provided by the position-dependent potential \( V(x) \) shown in the upper panels of figures 10 and 11. When \( \Gamma > \Gamma_c = 0.35 \) meV and \( \Delta V = 0 \), two Majorana bound states are localized near the ends of the wire (i.e., \( x \approx 0.2 \) \( \mu \)m and \( x \approx 2.2 \) \( \mu \)m, respectively), while for large \( \Delta V \) the wire is split into two disconnected segments, each of them hosting a pair of Majoranas. The behavior of the low-energy states in the intermediate regime is illustrated in figures 10 and 11. As a general feature, we note that states corresponding to small characteristic wavevectors (i.e., long-wavelength oscillations) tend to be contained in one of the two segments of the wire separated by \( \Delta V \). By contrast, states with large characteristic wavevectors (rapid oscillations) can more easily penetrate through the finite barrier. Furthermore, we note that Fermi \( k \)-vector \( k_F \) associated with the top occupied band increases with the Zeeman field, while the Fermi wavevectors corresponding to the lower energy bands are always larger than \( k_F \). Consequently, in the presence of a large barrier, the two pairs of Majoranas are characterized by a strong intra-pair hybridization and a weak inter-pair hybridization, which leads to two low-energy modes, mostly localized inside the \( L_{x1} \) and \( L_{x2} \) segments, respectively. The corresponding wavefunctions (states \( n = 1 \)—red line and \( n = 2 \)—yellow) are shown in figure 10. Reducing \( \Delta V \) (or increasing the Zeeman field) increases the inter-pair hybridization, which results in a lowest energy state with maxima near the ends of the wire (see figure 11).

The hybridization-induced splitting oscillations of the Majorana mode can be clearly seen in the field dependence

![Figure 10](image-url)
of the density of states (DOS), as shown in figure 12. We want to emphasize two features. First, regardless of the number of coupled Majorana pairs, only one mode exhibits zero-energy crossings at discrete values of the Zeeman field, which is a characteristic signature of Majorana physics in finite nanowires [157]. By contrast, the other low-energy mode is characterized by minima that vanish only in the limit $\Delta V \to \infty$, i.e., vanishing inter-pair tunneling. Second, the period and the amplitude of the oscillations induced by intra-pair hybridization increase with decreasing wire length approximately as $1/L_x$ [129]. Since $L_{x2} \approx 2L_{x1}$, the ratio between the corresponding periods and amplitudes is approximately two, as evident from the lower panel of figure 12. We note that, in very short wires (quantum dots), the period of the oscillations may be large, so that practically only one zero-energy crossing is accessible [157]. Also, in such quantum dot-superconductor structures the Coulomb interaction is expected to play an important role [165].

The characteristic signatures of the splitting oscillations in a set of two independent local measurements at the opposite ends of the wire, as reflected by the corresponding local density of states (LDOS), are shown in figure 13. Several features need to be emphasized. As discussed in section 4.2, the suppression of the gap closing signature stems from the spatial properties of various low-energy states. In short wires, there is no qualitative difference between extended states and states localized near the wire ends, and, consequently, a gap closing signature should be visible. This signature should be stronger at the left end of the wire, since the segment $L_{x1}$ is shorter. However, the corresponding features are rather weak (see figure 13) and could be very hard to resolve when on top of an incoherent in-gap background, such as that responsible for the soft gap observed experimentally [74–76]. In an actual experiment, the low-energy states couple to metallic states from the leads, while the states associated with low-energy bands are expected to have significant weight outside the

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Figure 11. Same as in figure 10, but for a lower value of the potential barrier $\Delta V$. Note that, unlike figure 10, the lowest energy state ($n = 1$, red line), corresponding to two overlapping Majorana bound states, is peaked near the ends of the wire for Zeeman fields associated with the topological SC phase.

Figure 12. Density of states as a function of the Zeeman field in the presence of a nonuniform potential with $\Delta V = 1$ meV (top) and $\Delta V = 2$ meV (bottom). Note the closing of the bulk gap at $\Gamma_0 \approx 0.35$ meV and the oscillations of the lowest energy modes for $\Gamma > \Gamma_0$. The corresponding LDOS at the opposite ends of the wire is shown in figure 13.

Figure 13. Splitting oscillations of the ZBCP as reflected by the LDOS at the left (L) and right (R) ends of the wire. The top two panels correspond to the parameters of figure 11, while the lower two panels are for the system illustrated in figure 10.
superconducting region of the wire [161]. This leads to broadening and could explain the soft gap observed in the experiments while hiding all the weak features that are present in figure 13. Consequently, we expect the splitting oscillations measured at the two ends of a wire containing a strong scattering center to be uncorrelated, as shown by the dominant low-energy features corresponding to \( \Delta V = 2 \) meV in figure 13. By contrast, in the presence of a weak scattering center (\( \Delta V = 1 \) meV in figure 13), the dominant low-energy features reveal the same ZBCP splitting at both ends of the wire. However, the amplitude of the splitting is strongly reduced because of the larger \( L_x \), and the oscillations may not be visible at finite energy resolution. Therefore, we conclude that the optimal experimental setup for observing correlated Majorana-induced splitting oscillations should use high-quality wires with \( L_x < 1 \mu\text{m} \).

5. Conclusions

The emergence of a zero-bias conductance peak above a certain critical value of the Zeeman field represents the necessary condition for the existence of zero-energy Majorana bound states in spin–orbit-coupled semiconductor–superconductor hybrid structures. Strong experimental evidence for signatures consistent with Majorana physics were recently reported in charge transport measurements on such nanowire heterostructures. These encouraging experimental developments have also raised a number of rather unexpected questions that need to be clarified before claiming victory. Nonetheless, corroborating these observations by performing a ‘smoking gun’ measurement, such as the proposed observation of the correlated splitting of the zero-bias peak, could be a step toward unambiguously establishing the existence of Majorana bound states in semiconductor nanowires. This goal could be achieved in the near future. In addition, a fractional AC Josephson effect, \( 2e^2/h \) quantized conductance through a MF state, or a signature of a Zeeman-tuned TQPT, say, by tunneling to a region away from the wire ends, can decisively establish the existence of MFs in semiconductor nanowire heterostructures.

However, the search for the non-Abelian Majorana fermion zero modes in semiconductor heterostructures is far from over. Future experiments have to address the sufficient conditions for the existence of the Majorana mode, which may consist of a tunneling-based interference measurement such as that discussed in section 2.8 or the direct observation of non-Abelian braiding statistics in some form. This direction will involve challenging experimental problems regarding the controlled engineering of complex devices, as well as basic aspects related to quantum decoherence and the manipulation of Majorana bound states. An important lesson provided by the recent developments is that, in real systems, key observable features are determined by various details of the structure, despite the topological nature of the superconducting state predicted to host the Majorana bound states. Therefore, to be able to discriminate between alternative scenarios and to clarify the mechanisms responsible for various features observed in the experiments, it is critical to develop realistic models of the heterostructures as discussed in section 3.

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Appendix A. Inter-band pairing and the ‘sweet spot’

In the ‘standard model’ of the Majorana nanowire, which involves a semiconductor (SM) wire with spin–orbit coupling, proximity-induced superconductivity, and Zeeman spin splitting, the emergence of zero-energy Majorana bound states requires values of the chemical potential consistent with an odd number of partially occupied sub-bands. As an example, let us consider the case illustrated in figure A.1, involving two bands, \( n = 1 \) and 2, and four values of the Zeeman field \( \Gamma \). The splitting between the pairs of sub-bands with opposite helicity (i.e., \( n^- \) and \( n^+ \)) is proportional to the applied field and, for \( \Gamma = \Gamma_0 \), the sub-bands \( 1^+ \) and \( 2^- \) are degenerate at \( k_0 = 0 \), \( \epsilon_{1^+} \) \( (0) = \epsilon_{2^-} \) \( (0) = \mu_2 \). The condition for the existence of a topological superconducting (SC) phase is satisfied for all four values of \( \Gamma \) when the chemical potential is \( \mu = \mu_1 \) (one partially occupied sub-band) or \( \mu = \mu_3 \) (three partially occupied sub-bands), but the system is topologically trivial when \( \mu = \mu_2 \) (two occupied sub-bands). This picture holds as long as the inter-band pairing is zero. However, when \( \Delta_{12} \neq 0 \), the number of partially occupied sub-bands does not represent a good criterion for establishing the topological nature of a given SC phase. More specifically, a quasi-1D nanowire with inter-band pairing and control parameters in the vicinity of the ‘sweet spot’ \( \Gamma = \Gamma_0 \) and \( \mu = \mu_2 \) is in the topologically nontrivial SC phase provided the inter-sub-band spacing \( |\epsilon_{1^+} - \epsilon_{2^-}| \) is smaller that the off-diagonal coupling \( \Delta_{12} \) [85]. In the limit of strong inter-band mixing, the sweet spot regime is characterized by a topological state that is robust against chemical potential fluctuations, such as those created by disorder. This stronger immunity can be understood in terms of the range of chemical potentials consistent with a topological SC state for a given value of the Zeeman field. Considering the example shown in figure A.1, for \( \Gamma = 0.4 \Gamma_0 \) there are two narrow topological regions (for chemical potentials in the vicinity of \( \mu_1 \) and \( \mu_3 \), respectively), separated by a topologically trivial phase. By contrast, for \( \Gamma \) sufficiently close to \( \Gamma_0 \), the range of \( \mu \) consistent with a topological SC state extends from the bottom of sub-band \( 1^- \) to the bottom of \( 2^+ \), without passing through any topological quantum phase transition.

How can inter-band mixing occur in SM nanowires with proximity-induced superconductivity? In essence, nonuniform interface tunneling generically induces inter-band coupling. Consider, for example, a hybrid structure containing a SC and a long SM nanowire with rectangular cross section with \( L_x \gg L_z \). The low-energy physics is controlled by the lowest energy transverse mode, \( n_z = 1 \), but, in general,
involves several $n_t$ bands. Now let us assume that only half of the nanowire is covered by the superconductor, so that $i(y) = \tilde{i}$ for $y < L_y/2$ and $i(y) = 0$ for $y > L_y/2$. Using equation (26), the effective SM–SC coupling becomes

$$\gamma_{n,n';}\ = \gamma_0 \sum_{i=1}^{N_z/2} \phi_n(i) \phi_{n'}(i), \quad \text{(A.1)}$$

where $\gamma_0 = v_F |\tilde{t}|^2 [\psi_1(i_{y})]^2$. The diagonal coupling is $\gamma_{n,n} = \gamma_0/2$, but, in addition, each band couples to all other bands of opposite parity. The inter-band couplings for neighboring bands, $n'_y = n_y \pm 1$, are comparable to the diagonal value, e.g., $\gamma_{12} \approx 0.85\gamma_1$. As described in section 3.3, the off-diagonal SM–SC coupling generates proximity-induced inter-band pairing, $\Delta_{n,n';}$, which leads to the sweet spot physics described above. Finally, we note that the experimental realization of nonuniform SM–SC coupling by partially covering the SM nanowire with superconductor [74] can provide additional benefits, such as reducing SC-generated screening and allowing gate-voltage control of the chemical potential.

**Appendix B. Projection of the effective tight-binding Hamiltonian onto a low-energy subspace**

To realize the projection of the effective tight-binding Hamiltonian onto a low-energy subspace, one needs to identify a convenient low-energy basis. While, in general, this problem has to be addressed using a combination of analytical and numerical tools, the 2-band lattice model described above has a simple analytical solution. Specifically, for an electron-doped nanowire with rectangular cross section and dimensions $L_x \gg L_y \sim L_z$, the single-particle quantum problem corresponding to $H_0$ from equation (18) has eigenstates $\psi_{n\sigma}(\tilde{i}) = \prod_{n=1}^{N_z} \phi_n(i_{y})\chi_{\sigma}$, where $n = (n_x, n_y, n_z)$ with $1 \leq n_i \leq N_i$, $\chi_{\sigma}$ is an eigenstate of the $\sigma_z$ spin operator, and

$$\phi_n(i_{y}) = \frac{2}{N_z + 1} \sin \frac{\pi n_y i_{y}}{N_z + 1}. \quad \text{(B.1)}$$

In equation (B.1) $\lambda = x, y, z$ and $L_{\lambda} = aN_{\lambda}$, where $a$ is the lattice constant. The eigenvalues corresponding to $\psi_{n\sigma}$ are

$$\epsilon_n = -2t_0 \left( \cos \frac{\pi n_x}{N_x + 1} + \cos \frac{\pi n_y}{N_y + 1} + \cos \frac{\pi n_z}{N_z + 1} + 3 \right) - \mu, \quad \text{(B.2)}$$

where $\mu$ is the chemical potential.

Next, we assume that only a few bands are occupied, and that the low-energy subspace is defined by the eigenstates satisfying the condition $\epsilon_n < \epsilon_{\text{max}}$, where the cutoff energy $\epsilon_{\text{max}}$ is typically of the order 100 meV. Using this low-energy basis, the matrix elements of the total Hamiltonian can be written explicitly, as described in [86]. The matrix elements of the SOI Hamiltonian from equation (18) are

$$\langle \psi_{n\sigma} | H_{\text{SOI}} | \psi'_{n'\sigma'} \rangle = \alpha \delta_{n,n'} \left[ q_{n,n'}(i \sigma_z) \delta_{n,n'} - q_{n,n'}(i \sigma_x) \delta_{n,n'} \right]. \quad \text{(B.3)}$$

The first term in equation (B.3) represents the intra-band Rashba spin–orbit interaction, while the second term couples different confinement-induced bands. Similarly, assuming that the Zeeman splitting $\Gamma$ is generated by a magnetic field oriented along the wire (i.e., along the $x$-axis), $\Gamma = g^* \mu_B B_x/2$, where $g^*$ is the effective $g$-factor for the SM nanowire, the matrix elements for the corresponding term in equation (15) are

$$\langle \psi_{n\sigma} | H_{\Gamma} | \psi_{n'\sigma'} \rangle = \Gamma \delta_{n,n'} \delta_{\sigma\sigma'}. \quad \text{(B.5)}$$

where $\sigma = -\sigma$. Adding together these contributions, the effective Hamiltonian describing the low-energy physics of the semiconductor nanowire in the presence of a Zeeman field becomes $H_{\text{eff}} = \langle \psi_{n}| H_{\text{SM}} + H_{\Gamma} | \psi_{n} \rangle$, with $\psi_n$ representing the spinor $|\psi_{n\uparrow}, \psi_{n\downarrow}\rangle$. Explicitly, we have

$$H_{\text{eff}} = \left[ \epsilon_n + \Gamma \sigma_z \delta_{n,n'} \right] + i \alpha \delta_{n,n'} \left[ q_{n,n'}(\sigma_y) \delta_{n,n'} - q_{n,n'}(\sigma_x) \delta_{n,n'} \right], \quad \text{(B.6)}$$

where $n = (n_x, n_y, n_z)$, $\epsilon_n$ is given by equation (B.2) and $q_{n,n'}$ by equation (B.4). Note that a similar effective low-energy Hamiltonian can be written for an infinite quasi-1D wire.
In the limit $L_x \to \infty$, the wavevector $k_x$ becomes a good quantum number and we have

$$H_{nn'}(k_x) = [\epsilon_n(k_x) + \alpha_R k_x \sigma_x + \Gamma k_x \sigma_y] \delta_{nn'} - i\alpha \delta_{n'n} \sigma_z \delta_{n'n},$$

where $\alpha_R = \alpha a$ and $n = (n_x, n_z)$ labels the confinement-induced bands with energy

$$\epsilon_n(k_x) = \frac{h^2 k_x^2}{2m^*} - 2t_0 \left( \cos \frac{\pi n_y}{N_y} + \cos \frac{\pi n_z}{N_z} - 2 \right) - \mu. \quad (B.8)$$

**Appendix C. Proximity effect in hole-doped semiconductors**

To illustrate the dependence of the SC proximity effect on the details of the SM–SC coupling, we consider the case of hole-doped SM nanowires. We use the 4-band Luttinger-type model defined by equations (20) and (21) to describe a hole-doped SM nanowire with rectangular cross section proximity-coupled an s-wave SC. We assume that the z axis is perpendicular to the interface and corresponds to the proximity-coupled an s-wave SC. We assume that the $z$ axis is perpendicular to the interface and corresponds to the (0, 0, 1) crystal axis of the underlying fcc lattice. The specific form of the SM–SC coupling Hamiltonian (23) depends on the symmetry of the localized states that define the effective SC Hamiltonian (22). Assuming that $\mu_{sc}$ lies within a band with s-type character, we notice that the orbitals that are responsible for the coupling across the interface are the $|z\rangle$ orbitals. Consequently, only the $\Phi_{\pm \frac{1}{2}}$ eigenstates couple to the SC. The corresponding matrix elements in equation (23) can be written as

$$i_{k|j\rangle}^{\pm \frac{1}{2} \sigma} = \sqrt{\frac{\pi}{2}} \delta_{i\nu} d_{j\delta} \delta_{\sigma \sigma'}, \quad (C.1)$$

where $\frac{1}{2} = \pm \frac{1}{2}$ and $i$ is a constant, while the coupling of the 3/2 states vanishes, $i_{k|j\rangle}^{\pm \frac{3}{2} \sigma} = 0$. We address the following question: what is the consequence of this selective coupling on the strength of the proximity effect in hole-doped nanowires with rectangular cross section? Specifically, we focus on the effective SM–SC coupling $\gamma_c$ for the top valence band.

To determine the effective coupling, we calculate numerically the wavefunctions $\Psi_{\pm}$ corresponding to the double degenerate top valence band at $k_x = 0$. These states can be expressed as four-component spinors, $\Psi_{\pm}(i_\nu, j_\delta) = \begin{pmatrix} \psi_1^{(s)} & \psi_2^{(s)} & \psi_3^{(s)} & \psi_4^{(s)} \end{pmatrix}^T$, and we have

$$\gamma_c = \frac{1}{2} \nu \nu' \sum_{i_j=1}^{N_t} |\psi_3^{(s)}(i_j, i_0)\rangle|^2. \quad (C.2)$$

For comparison, in the case of an electron-doped wire with uniform tunneling across the SM–SC interface, the effective coupling of the lowest conduction band can be obtained from equation (26) for $i(i_0) = i$ and $n = n' = (1, 1, 1)$. We have $\gamma_c = \nu \nu' |\phi_1^{(s)}(i_0)|^2 \approx 2\pi^2 \nu \nu' |\phi_1^{(s)}|^2 / (N_t + 1)^3$. Note that $\gamma_c$ is independent of the wire width $L_x$ and decreases approximately as $1/L_x^3$ with increasing wire thickness $L_x$.

due to the decrease of the wavefunction amplitude at the interface. By contrast, the effective coupling of the top valence band is characterized by a strong dependence on $L_y$ for a fixed wire thickness $L_x$. The numerical results are shown in figure C.1. Note that in the quasi-2D limit, $L_y \to \infty$, the effective coupling of the top valence band to the bulk SC vanishes. This can be understood by noticing that the top valence band of a SM slab is a purely heavy-hole band and, for a $(0, 0, 1)$ surface orientation, the corresponding states have vanishing $\psi^{(s)}_{\pm \frac{1}{2}}$ components. Consequently, we conclude that no proximity-induced superconductivity can occur in the top valence band of planar SM–SC heterostructures with a $(0, 0, 1)$ interface. This result holds for different interface orientations. Nonetheless, in quasi-1D nanowires, the top valence band is a superposition of heavy-hole and light-hole states and, consequently, the effective coupling to the SC is non-zero, as shown in figure C.1. Note that the amplitude of the light-hole component varies non-monotonically with $L_y$ and has a sharp discontinuity for a width-to-thickness ratio $L_y/L_x \approx 2$. A quantitative description of the SC proximity effect in hole-doped nanowires requires a more detailed modeling of the wire (e.g., using the 8-band model).

**Appendix D. Proximity effect in multiband systems and the collapse of the induced gap**

We illustrate the role of multiband physics in proximity-coupled finite-size systems by calculating the low-energy spectrum of a SM thin film—SC slab heterostructure with uniform coupling across the planar interface. This allows us to focus on the proximity-induced inter-band coupling involving bands with different $n_z$ quantum numbers, a problem that was not previously investigated in the literature. First, we consider the limit $\Delta E_{nn'} \gg \Delta_0$ and we test the accuracy of the static approximation that allows us to define the effective Hamiltonian (31). For simplicity, the SM film is described using the 2-band model with nearest-neighbor hopping.
The static approximation energies within the SC gap—except near the gap edge, where that the effective Hamiltonian description is highly accurate at the results are shown in the lower panel of figure D.1. Note compared with the solution of the full BdG equation (28).

The effective Hamiltonian is constructed using the decoupled band approximation and the corresponding low-energy spectrum is approximated. The fully decoupled band approximation fails, as the inter-band gaps are now comparable to $\Delta_0$ (see the upper panel of figure D.2). In particular, inter-band coupling results in a collapse of the induced SC gap. A detailed analysis of this effect is presented in [145]. We emphasize that this effect is not due to the decrease of the wavefunction amplitude at the interface with increasing $N_z$, as this is compensated for by increasing the transparency of the interface, i.e., $\gamma_0$, but rather stems from the off-diagonal elements of the effective coupling matrix $\gamma_{n,n'}$. Also, we note that in this regime the construction of the effective Hamiltonian (31) has to involve the high-energy bands, as they are intrinsically coupled to the low-energy bands and renormalize them strongly, which ultimately leads to the collapse of the induced SC gap.

Appendix E. Low-energy states in the presence of disorder

We illustrate some of the generic features of low-energy BdG spectrum of a disordered SM–SC hybrid system by considering a SM nanowire of length $L_x = 3$ $\mu$m and rectangular cross section with $L_y = 80$ nm and $L_z = 40$ nm in the presence of a disorder potential $V(r) = V_0 f_V(r)$, where the disorder profile is described by the random function $f_V$ with $|f_V(r)| \leq 1$ and $V_0$ represents the amplitude of the

$\begin{align*}
N_z &= 40 \\
N_z &= 80
\end{align*}$
disorder potential. The low-energy spectrum is calculated using a 2-band model, as described in section 3.1. All the calculations are done for a specific disorder realization, i.e., a fixed profile $f_V$, but for variable disorder strength $V_d$. First, we consider a system with three partially occupied bands (five spin sub-bands) in the presence of a Zeeman splitting $\Gamma = 0.6$ meV and a fixed chemical potential $\Delta \mu = 0$, as measured relative to the bottom of the third band in the absence of Zeeman splitting. The clean wire ($V_d = 0$) is in the topological SC phase that supports zero-energy Majorana bound states. The corresponding BdG spectrum is shown in the top panel of figure E.1 (black circles and red diamonds for the Majorana states). In the presence of disorder ($V_d \neq 0$), the minigap that protects the Majorana bound state becomes smaller and, eventually, collapses. The dependence of the non-zero lowest energy modes on the strength $V_d$ of the disorder potential is shown in the bottom panel. We note that, in the presence of disorder, multiple zero-energy modes are possible as disorder effectively cuts the wire into disconnected topologically nontrivial segments supporting Majorana bound states at their ends. Typically, these segments are relatively short and the states localized at the ends of each segment (which can be viewed as representing a Majorana chain) overlap significantly and are characterized by near-zero energies that oscillate with the chemical potential and the Zeeman splitting.

A similar proliferation of low-energy states with increasing strength of the disorder can be seen in a system with parameters corresponding to the trivial SC phase, as shown in figure E.2. Note that in this case the decrease of the quasiparticle gap with $V_d$ is slower than that corresponding to $\Delta \mu = 0$. This behavior can be understood qualitatively by noting that disorder tends to localize the low-energy states and that this effect depends on the characteristic Fermi wavevector associated with those states. Increasing $\Delta \mu$ corresponds to larger values of $k_F$ and to a weaker localization. This behavior is illustrated by the profiles of the low-energy states shown in figure E.3. The low-energy states corresponding to $\Delta \mu = 0$ exhibit stronger localization that those for $\Delta \mu = 3$ meV, in spite of the smaller amplitude of the disorder potential. We note that the low-energy states associated with the low-energy bands are characterized by large values of $k_F$ and, consequently, are harder to localize. Finally, we note that the other key parameter that controls the effect of disorder on the low-energy states is the Zeeman splitting. Increasing $\Gamma$, which breaks time-reversal symmetry, facilitates the collapse of the SC gap. Again, this effect is stronger for states with low values of the characteristic $k_F$ which typically corresponds to the top occupied band, although significant band mixing is possible for certain types of disorder. Consequently, in a wire with hard confinement, the near-zero-energy states with most of the spectral weight coming from low-energy bands require higher values of the Zeeman splitting than the disorder-induced near-zero-energy states associated with the top band. On the other hand, the energy of these states can become exponentially small even in the absence of disorder.
Figure E.3. Position dependence of the amplitude of the lowest energy states for a wire with $L_x = 3 \, \mu m$ and $\Gamma = 0.6 \, meV$. The top panel corresponds to a clean wire in the topological SC phase. The red line with maxima near the ends of the wire represents the Majorana bound states. In the presence of disorder, all the states become localized in various regions of the wire. The wavefunction of the lowest energy state of clean wire ($V_d = 0$) in the topological trivial state is characterized by an envelope with maxima near the ends of the wire and oscillations corresponding to a certain value of $k_F$. The lowest energy states associated with the low-energy occupied bands (not shown) have similar characteristics, but higher values of $k_F$. For given values of the disorder strength and Zeeman splitting, states with larger characteristic Fermi wavevectors (shorter oscillation period) exhibit weaker localization.

if the confinement potential is smooth [110]. Furthermore, the states associated with low-energy bands can penetrate through finite potentials and extend into the normal section of the wire [161].

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