1. Introduction

In the quest for a topological quantum computer [1, 2], the intense investigation of topological phases of matter [3–5] has propelled the elusive Majorana fermion [6] to the center of a variety of physical systems that enables the exploitation of its non-Abelian properties [7, 8]. One of the most promising schemes for engineering the topological superconducting phase that hosts zero-energy Majorana bound states [9–12] involves a semiconductor (SM) with strong spin-orbit coupling in the presence of an applied Zeeman field and proximity-coupled to an s-wave superconductor (SC) [13–16].

The recent experimental realization of the one-dimensional (1D) version of this proposal [15, 16] in semiconductor–superconductor hybrid structures—the so-called Majorana wire—has generated reports of signatures consistent with the presence of zero-energy Majorana bound states, such as the fractional Josephson effect [17] and the emergence of a zero-bias peak in the differential conductance [18–22]. However, these encouraging experimental advances have also underscored a series of discrepancies between predicted and observed features, as well as potential problems [23], most notably the soft gap that characterizes the proximity-induced superconductivity in SM nanowire-SC hybrid structures [18, 24, 25] and the absence of any signature associated with the closing of the quasiparticle gap [18, 26] at the topological quantum phase transition (TQPT) [9]. Moreover, the possibility that observable features similar to those generated
by Majorana bound states can appear in the topologically trivial phase due to, e.g., strong disorder [27–30] or soft confining potentials [31], or Kondo physics [32] has not been clearly eliminated. Zero-bias anomalies have been recently related to parity crossings of Andreev levels and regarded as precursors of Majorana modes in short nanowires [33].

In general, while the Majorana bound states are expected to emerge in a topological SC phase and, consequently, to enjoy a certain degree of protection against small perturbations, the stability of the Majorana mode as well as some of the observable features that it generates [18–22] depend critically on certain details of the system, such as disorder, multiband occupancy, finite size effects [34, 35], barrier potentials, and the strength of the effective coupling between the SM wire and the SC and between the wire and the metallic lead [23]. In this context, it becomes critical to incorporate the effects of the Coulomb interaction using approaches that are both reliable and simple enough to accommodate these influences.

Electron–electron interactions are expected to affect the stability of the Majorana modes [36–42] by renormalizing the induced SC pairing potential and the characteristic length scale of the zero-energy bound states [36]. Under strong interaction, a complete suppression of the induced SC pair potential can occur [36, 37], along with an increase in the localization length of the Majorana modes [39]. The interplay between disorder and interaction in Majorana wires was also predicted to favor a quantum phase transition from a topological SC phase to a topologically trivial localized phase [40]. At the same time, the presence of interactions was found to broaden the chemical potential range that supports the topological SC phase [39], thus enhancing the immunity of the Majorana modes against local fluctuations of the chemical potential. A broadening of the chemical potential window for Majorana modes has also been predicted for a different physical set-up, based on an array of superconducting islands with mutual interaction [41].

In nanowires, the effect of interactions is enhanced by the effective low dimensionality of the system. Consequently, it was found that in multiband nanowires the phase boundaries in the Zeeman field—the chemical potential plane—are renormalized [38]. Further, the transport properties of a nanowire having a structure similar to that used in recent experiments [18], i.e. with part of the wire’s length proximity-coupled to the SC and a normal segment serving as a lead, have been studied [43] by treating the system as a superconductor-Luttinger liquid junction. Finally, repulsive interactions were recently predicted [44] to drive a mechanism that results in the reversal of the sign of the effective pair potential in the wire and the emergence of time-reversal invariant topological superconductivity [45–54].

Existing studies have included interaction effects using a variety of approaches ranging from the Hartree–Fock approximation to bosonization and the density-matrix renormalization group technique. While some of these methods can accurately account for the effects of interactions, they have serious limitations when key characteristics of the system, such as the finite wire thickness or various details of the SC proximity effect [23], are incorporated into the theoretical description.

In this paper we study a standard Majorana wire configuration—a semiconductor wire proximity-coupled to a superconductor in the presence of a repulsive $\delta$ function interaction that realistically describes a strongly screened regime. In the standard many-body manner, we incorporate this interaction in a Hartree–Fock-type approximation of the Bogoliubov–de Gennes (BdG) Hamiltonian that can be reliably used to account for the effects of Coulomb interaction as well as other experimentally relevant features, such as the finite length of the wire. Within this formalism we calculate the Majorana states in a flat, two-dimensional quantum wire of both finite and infinite length. We emphasize that this formalism can be naturally expanded to incorporate finite range interactions and experimentally relevant conditions, such as gate-induced and disorder potentials. Our calculations show that in the finite wire the modes increase their localization length, while for an infinite wire the phase diagram describing transitions to a topological superconductor phase in terms of chemical potential and Zeeman energy depends on the strength of the Coulomb interaction. On account of the interaction, for a fixed Zeeman energy the phase boundaries are pushed to higher chemical potentials, whereas for a fixed chemical potential the boundaries can shift either to lower or to higher Zeeman energies. However, when the Zeeman energy is large enough such that the spins are fully polarized along the magnetic field, the phase boundaries do not depend on the interaction strength.

The outline presented above is reflected by the structure of this paper. We first describe the physical model, then the effective BdG Hamiltonian which includes the Coulomb interaction, then the results for the finite and infinite wire. Finally a cumulative summary of conclusions is presented.

2. The model

The following considerations are based on the standard model of a thin Majorana-wire of width $L_y$ and length $L_x$ placed in a magnetic field $B_z$ oriented along the y direction, i.e. parallel to the wire, that induces a Zeeman splitting, as shown in figure 1. The wire is strongly confined in the z direction, i.e. $L_z \ll L_x$, such that only the lowest mode in the z direction is relevant for the electronic states. The SM wire is endowed with a Rashba spin–orbit interaction (SOI) linear in the electron momentum, and of strength $\alpha$.

The single particle Hamiltonian of an electron of momentum $\mathbf{p}$ and spin $\sigma$ is consequently written as

\begin{align}
H = & \sum_{\mathbf{k},\sigma} \left( \varepsilon_{\mathbf{k}} \uparrow \downarrow + \varepsilon_{\mathbf{k}} \downarrow \uparrow \right) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \\
+ & \sum_{\mathbf{k},\sigma} \left( \varepsilon_{\mathbf{k}} - \Delta_0 \right) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\bar{\sigma}} + \frac{\Delta_0}{2} \left( \uparrow \Sigma \downarrow - \downarrow \Sigma \uparrow \right)
\end{align}

Figure 1. The physical system: a semiconductor quantum wire is built on the surface of a metallic s-wave superconductor. The superconductivity is induced in the wire by proximity effect. The wire is quasi-two-dimensional, with the thickness $L_z$ being much smaller than the width $L_y$, which is much smaller than the length $L_x$. An external longitudinal magnetic field $B_z$ is used to create a Zeeman splitting.
\[ H = \frac{p^2}{2m} + \sigma_z B + a (\sigma_x p_x - \sigma_y p_y). \]  
\[ (1) \]

The boundary conditions are set by hard-walls at \( x = \pm L_x/2 \) and \( y = \pm L_y/2 \). We use the basis generated by the single particle eigenstates of \( H_0 = p^2/2m \), labeled by \( q \), and described as \( |q\rangle = |n_x,n_y\rangle \), or \( q_p(x) = \varphi_{n_x, n_y}(x) |s\rangle \), where \( n_x, n_y \) are positive integers, \( s \) is the spin projection along \( z \), and
\[ 
\varphi_{n_x, n_y}(x) = \frac{2}{L_x} \sin \left( \frac{n_x(x+L_x/2)}{L_x} \pi \right), \\
\varphi_{n_x, n_y}(y) = \frac{2}{L_y} \sin \left( \frac{n_y(y+L_y/2)}{L_y} \pi \right). 
\]  
\[ (2) \]

In order to simplify notations the same symbol \( \varphi \) is used for the 1D wave functions corresponding to \( x \) and \( y \) directions, and for the basis vector as well.

When proximity-coupled to a superconductor the wire is described by a many-body Hamiltonian written in terms of the single-particle creation and destruction operators \( c_i^\dagger \) and \( c_i \) associated with the basis states (3) [55],
\[ \hat{K}_S = \sum_{q,q'} \left( (H_{qq'} - \mu \delta_{qq'}) c_i^\dagger c_i + \frac{1}{2} \left( \Delta_{qq'} c_i^\dagger c_{i'} + \text{h.c.} \right) \right). \]  
\[ (3) \]

In equation (3) the proximity-induced superconductivity is described by the pairing potential \( \Delta \) with matrix elements \( \Delta_{qq'} = \delta_{n_i n_{i'}} \delta_{\Delta_{\epsilon \epsilon'}} \Delta_\epsilon, \) where \( |q\rangle = |n_x,n_y\rangle \) and \( |q'\rangle = |n'_x,n'_y\rangle \).

Within the spin space \( \Delta_{\epsilon \epsilon'} = \Delta_{\epsilon \epsilon'} = 0 \) and \( \Delta_{\epsilon \epsilon'} = -\Delta_{\epsilon \epsilon'} = \Delta, \) which is the pairing energy in the induced superconductor. \( H_{qq'} \) represents the matrix elements of Hamiltonian (1) and \( \mu \) denotes the chemical potential.

In addition to the attractive pairing induced through the proximity effect, the electrons in the wire also experience a purely repulsive Coulomb interaction (3),
\[ \hat{V} = \frac{1}{2} \sum_{q,q',q''} V_{qq',qq''} c_i^\dagger c_{i'} c_{i''} c_i, \]

containing the matrix elements of the Coulomb potential
\[ V_{qq', qq''} = \frac{1}{2} \sum_{q,q',q''} V_{qq',qq''} \left| u_{q}(\mathbf{r} - \mathbf{r}') \right| \left| p_{q''} \right| \]
\[ = \int d\mathbf{r} d\mathbf{r}' \varphi_{q}^\dagger (\mathbf{r}) \varphi_{q'}^\dagger (\mathbf{r}') u(\mathbf{r} - \mathbf{r}') \varphi_{p'} (\mathbf{r}') \varphi_{p} (\mathbf{r}). \]  
\[ (5) \]

On account of the proximity to the superconductor the Coulomb electron–electron repulsion is expected to be strongly screened, suitably described by a delta function, with \( u_0 \) as a sample specific parameter. As described in the Appendix, \( u_0 \) is estimated to be of the order of some \( eV \text{nm}^2 \).

In the reference basis (3), the matrix elements of the Coulomb potential can be calculated analytically. With \( |q\rangle = |n_x,n_y\rangle \), \( l(q') = |n'_x,n'_y\rangle \), \( l(p') = |n''_x,n''_y\rangle \), we obtain
\[ \delta_{\epsilon \epsilon'} = \sum_{n_i, n_{i'}} \left( \Delta_{\epsilon \epsilon'} c_i^\dagger c_{i'} + \text{h.c.} \right), \]

\[ \text{where} \]
\[ K(n_i, n_{i'}, m_i, m_{i'}) \]
\[ \Delta_{\epsilon \epsilon'} = \sum_{n_i, n_{i'}, n_m, n_{m'}} \left( \delta_{\epsilon \epsilon'} \delta_{\epsilon \epsilon'} + \Delta_{\epsilon \epsilon'} (\epsilon_{n_{i'}} - \epsilon_{n_{i'}}) + \text{h.c.} \right). \]  
\[ (7) \]

\[ (8) \]

3. The effective BdG Hamiltonian

The spectrum of quantum states of the superconducting wire is found by rewriting the original Hamiltonian via canonical transformations of the field operators [56, 57]. Although the derivation of the BdG Hamiltonian is textbook material [58], we prefer to summarize it here for clarity. The Bogoliubov operators for the creation and destruction of an excited state with energy \( \epsilon, \gamma' \) and \( \gamma \) are introduced. These satisfy the Fermionic anticommutation rules, i.e.
\[ \{ \gamma, \gamma' \} = \delta_{\epsilon \epsilon'}, \]  
\[ \{ \gamma, \gamma' \} = \{ \gamma, \gamma' \} = 0, \]

while satisfying the particle-hole symmetry, \( \gamma' = \gamma \). Operators \( c_i \) are expanded as
\[ c_i = \sum_{c > 0} (u_{iq}c^\dagger + v_{iq}c^\dagger), \]  
\[ c_i = \sum_{c > 0} (u_{iq}c^\dagger + v_{iq}c^\dagger), \]

where \( u_{iq} \equiv \{ c_i, \gamma' \} \) and \( v_{iq} \equiv \{ c_i, \gamma \} \) are numerical (complex) coefficients to be determined. Equation (10) are inserted in the Hamiltonian (3) where the \( \gamma' \)s are subsequently rearranged in the normal order (creation part to the left, destruction part to the right, and a negative sign for an odd number of permutations), using Wick's theorem [56]. In the simplest case of only two operators one obtains, for example,
\[ c_i^\dagger c_i = \langle c_i^\dagger c_i \rangle = c_i^\dagger c_i + c_i^\dagger c_i, \]  
\[ \text{and the contraction (second term) can easily be calculated by taking the expectation value on the vacuum of the } \gamma' \text{s, } \gamma(0) = 0. \]

The expected value of the normal product is zero, and hence
\[ c_i^\dagger c_i = \sum_{c > 0} v_{iq}c^\dagger, \]  
\[ c_i^\dagger c_i = \sum_{c > 0} u_{iq}c^\dagger, \]  
\[ c_i^\dagger c_i = \sum_{c > 0} u_{iq}c^\dagger, \]

After calculating the normal (N) products, the Hamiltonian (3) becomes
\[ \hat{K}_S = E_0 + \sum_{c > 0} \left[ h_{cc'}^{(1)} \gamma c^\dagger + \frac{1}{2} \Delta_{\epsilon \epsilon'} (\epsilon_{c'} - \epsilon_{c'} + \text{h.c.} \right) \].  
\[ (11) \]

where the following notations have been used: \( h_{cc'}^{(1)} = \sum_{q, q'} H_{qq'} u_{cq} \).

\[ E_0 = \sum_{c > 0} \left[ h_{cc'}^{(2)} \gamma c^\dagger + \frac{1}{2} \Delta_{\epsilon \epsilon'} (\epsilon_{c'} - \epsilon_{c'} + \text{h.c.} \right) \].  
\[ (12) \]

\[ E_0 = \sum_{c > 0} \left[ h_{cc'}^{(2)} \gamma c^\dagger + \frac{1}{2} \Delta_{\epsilon \epsilon'} (\epsilon_{c'} - \epsilon_{c'} + \text{h.c.} \right) \].  
\[ (13) \]
\[ E_0 \] is the ground-state energy of the superconductor condensate in the quantum wire. \( h_{\epsilon}^{(1)} \) contains the spectrum of excitations which can be rewritten as

\[ h_{\epsilon}^{(1)} = \sum_{q,\epsilon} \left( \frac{\epsilon}{2} + \frac{1}{2} \Delta_{q} \left( \Psi^\dagger_{q} \Psi_{-q} - \Psi_{q} \Psi^\dagger_{-q} \right) \right) \]

where \( \epsilon \) and \( \Psi \) can be seen as particle/hole (or isospin) components of a combined wave vector \( \Psi = \Psi_{q} \), which define the so-called Nambu space. The central matrix is known as BdG Hamiltonian

\[ H_{\text{BdG}} = \begin{pmatrix} \frac{\epsilon}{2} + \frac{1}{2} \Delta_{q} & \Delta_{q} \\ -\Delta_{q} & -\frac{\epsilon}{2} \end{pmatrix} \]

If \( |\Psi_{q} \rangle \) is an eigenvector of \( H_{\text{BdG}} \) with eigenvalue \( \epsilon \) then one can show [56, 57] that \( h_{\epsilon}^{(2)} = 0 \). This means that the excitation spectrum of the quantum wire in the superconductive state is the spectrum of \( H_{\text{BdG}} \).

Similarly, the two-particle interaction in (3) is subjected to the canonical transformation, leading to four \( \gamma \) operator products [57]. In this case of Coulomb interaction Wick's theorem gives,

\[ c_{q}^{\dagger} c_{p}^{\dagger} c_{p} c_{q} = N_{2} + N_{2} + N_{0} \]

where \( N_{2} \) is the normal product with no contraction, \( N_{2} \) is the sum of all combinations with only one pair of \( \Gamma \) 's contracted, and \( N_{0} \) is the sum with two pairs contracted. \( N_{0} \) is only a c-number and has a contribution to the energy of the condensate \( E_{0} \), \( N_{2} \) has combinations of four \( \Gamma \) operators which can be interpreted as Coulomb correlations of a higher order than \( N_{2} \) and which will be neglected. We are thus left with \( N_{2} \),

\[ N_{2} = N_{2}^{(2)} + N_{2}^{(3)} + N_{2}^{(4)} + N_{2}^{(23)} + N_{2}^{(24)} + N_{2}^{(34)} \]

where the upper indices of each term indicate the contracted operators:

\[ N_{2}^{(2)} = N(c_{q} c_{q}^{\dagger} c_{p} c_{p}^{\dagger}) = \sum_{\epsilon>0} \epsilon_{\epsilon} N(c_{\epsilon}^{\dagger} c_{\epsilon}) \]

\[ N_{2}^{(3)} = N(c_{q}^{\dagger} c_{q} c_{\epsilon}^{\dagger} c_{\epsilon}) = -\sum_{\epsilon>0} \epsilon_{\epsilon} N(c_{\epsilon}^{\dagger} c_{\epsilon}) \]

After the remaining \( N \) products are calculated and inserted (4), the coefficient of \( \gamma_{\epsilon}^{\dagger} \), are identified and added to \( h_{\epsilon}^{(1)} \). The changes of the BdG Hamiltonian due to the Coulomb contributions are:

\[ H_{\epsilon_{\epsilon}}^{(2)} \rightarrow H_{\epsilon_{\epsilon}} + W_{\epsilon_{\epsilon}}^{\dagger} \gamma_{\epsilon_{\epsilon}}^{\dagger} \rightarrow H_{\epsilon_{\epsilon}} + \Delta_{\epsilon_{\epsilon}} + I_{\epsilon_{\epsilon}} \]

where

\[ W_{\epsilon_{\epsilon}} = \sum_{\epsilon>0} \epsilon_{\epsilon} N(c_{\epsilon}^{\dagger} c_{\epsilon}) \]

\[ I_{\epsilon_{\epsilon}} = \frac{1}{2} \sum_{\epsilon>0} \epsilon_{\epsilon} N(c_{\epsilon}^{\dagger} c_{\epsilon}) \]

In the derivation of these results the symmetry properties of the Coulomb matrix elements have been used: \( V_{q,p}^{\dagger} = V_{q,p}^{\dagger} = V_{q,p}^{\dagger} \). We obtain \( W_{\epsilon_{\epsilon}} = W_{\epsilon_{\epsilon}}^{\dagger} \) and
\[ \Gamma_{qq'} = -\Gamma_{q'q}, \text{in agreement with the similar symmetries of the non-Coulomb term.} \]

On account of the electron-hole symmetry we also write,
\[ \sum_{\nu} v_{\nu} v_{\nu}^* = \sum_{\nu} u_{\nu} u_{\nu}^*, \]

the restriction to negative \( \epsilon \) corresponding to the occupied particle states of the original quantum wire in the normal state, i.e. below the chemical potential. The new matrices \( W \) and \( \Gamma \) depend themselves on the eigenstates of the BdG Hamiltonian. Therefore, to solve the new eigenvalue problem, i.e. with Coulomb contributions, an iterative numerical scheme is implemented.

4. Results

4.1. The quantum wire of finite length

We consider a quantum wire of width \( L_x = 100 \text{ nm} \) and length \( L_y = 5000 \text{ nm} \), and neglect the thickness \( L_z \). We note that this geometry represents a good approximation for thin nanoribbons, provided only one transverse mode (i.e. one confinement-induced band associated with the \( z \)-direction) is occupied. The material parameters are those of InSb: \( m_{\text{eff}} = 0.016, g_{\text{eff}} = -50, \) and \( \alpha = 20 \text{ meV nm} \). The energy spectrum of the spinless, normal wire, without Coulomb interaction, is
\[ E_{\text{spinless}} = \left( \hbar^2 \pi^2 / 2 m_{\text{eff}} \right) \left( (n_x / L_x)^2 + (n_y / L_y)^2 \right). \] (21)

In the presence of a magnetic field of strength \( B \) the Zeeman energy (i.e. the Zeeman splitting) in meV is
\[ E_{z} = |g_{\text{eff}}| \mu_B B = 2.9 \times B \text{[T]}. \] (In other papers the Zeeman energy may be defined as \( E_z = 1/2 |g_{\text{eff}}| \mu_B B \).)

The superconductor parameter is fixed to \( \Delta = 0.25 \text{ meV} \). The BdG Hamiltonian is diagonalized numerically in the space covered by the basis \( \{ \Psi_{\gamma} \} = \{ \Psi_{n_x n_y s} \} \) with \( s = \pm 1 \) the Nambu quantum number. In the following examples we use \( n_x \leq 4 \) and \( n_y \leq 100 \), such that the size of the basis is \( 2 \times 100 \times 4 \times 2 = 1600 \).

In figure 2 we show BdG spectra without and with Coulomb repulsion. Only the central part of the spectra is shown in the figures, corresponding to the low-energy excitations. In the absence of a magnetic field and Coulomb interaction the induced superconductor gap of \( 2\Delta = 0.5 \text{ meV} \) is clearly visible in the spectrum shown in figure 2(a). As expected, the gap decreases in the presence of the Coulomb repulsion, and with \( u_0 = 4 \text{ eV nm}^2 \) the new gap is \( 0.23 \text{ meV} \). We note that this reduction of the induced SC gap represents a more meaningful measure of the Coulomb effects than the magnitude of the coupling constant \( u_0 \) itself.

As the strength of the magnetic field along the wire \( B_y \) increases, the superconductor gap disappears at a certain field value corresponding to a TQPT, followed by a reemergence as the system enters a topological superconductor phase with two Majorana zero-energy states, localized at the two ends of the wire. In the absence of the Coulomb interaction, if the Fermi energy is at the bottom of an energy band of the normal wire, for example \( \mu = E_{\text{g}} = 9.4 \text{ meV} \), the gap closes when the Zeeman energy is equal to the induced superconductor gap, \( E_z = 2\Delta \), i.e. for \( B_y = 0.17 \text{ T} \). In figure 2(b) we consider a slightly stronger magnetic field, \( B_y = 0.3 \text{ T} \), for which the gap is open again, and two zero-energy Majorana bound states are created in the middle of the gap. Within our basis these states are ranked as 800 and 801 on the energy scale. In the interacting case, the system is still in the topologically trivial phase, but the quasiparticle gap will close at a higher field \( B_y = 0.5 \text{ T} \) (not shown).

At an even higher field, for example \( B_y = 0.68 \text{ T} \), Majorana states are obtained both with and without interaction, figure 2(c). The probability distributions of these states are shown for comparison in figure 3. As expected, the localization effect at the ends of the wire is reduced by the interaction, but it is still present and consistent with states created inside the energy gap. Note that the double peak structure of the Majorana modes is due to the fact that these states are associated with the top occupied band, which, for the parameters used in the calculation, corresponds to \( n_x = 2 \). Next, in figure 2(d) we keep the same magnetic field, but increase the Fermi energy into the second band to \( \mu = 10.6 \text{ meV} \), i.e. by \( \delta \mu = 1.2 \text{ meV} \). The results are now opposite to figure 2(b), with the Majorana present in the interacting case, but absent for \( u_0 = 0 \), as \( E_z < 2\sqrt{\delta \mu^2 + \Delta^2} \), i.e. the wire is in the topologically trivial phase.

4.2. The quantum wire of infinite length

For the infinite wire, the basis functions in the \( y \) direction \( (3) \) become plane waves with wave vectors \( k \). For any fixed \( k \), which is here a good quantum number, the eigenstates can be labeled with \( |q\rangle = |n_x s \rangle \). The BdG Hamiltonian is now diagonal in \( k \), and therefore the matrix elements of the Coulomb terms \( W \) and \( \Gamma \), equations (19) and (20), become \( W_{qq'} (k) \) and \( \Gamma_{qq'} (k) \).

In figure 4 we show energy spectra for a quantum wire of infinite length and of width \( L_x = 100 \text{ nm} \), without Coulomb interaction, both in the normal state and at the transition to the topological superconductor state occurring at minimum magnetic field, i.e. for \( E_z = 2\Delta \), when the energy gap is closing for \( k = 0 \) [59]. For a slightly higher magnetic field, like \( B_y = 0.3 \text{ T} \), the gap reopens and the resulting BdG spectra are shown in figure 5(a), both with and without Coulomb interaction, to be compared with the versions obtained for the finite wire and shown in figure 2(b). Consistent with the finite wire calculation, for \( B_y = 0.3 \text{ T} \) the
system is in the topological SC phase in the absence of interaction, but still in the topologically trivial phase for $u_0 = 4 \text{ eV nm}$.

The gap obtained for the BdG spectrum of the infinite wire with interaction is 0.43 meV, which is slightly higher than the analogous result seen in figure 2(b) for the finite wire of length 5000 nm, which is 0.20 meV, i.e. the energy difference between the states 800 and 801. Hence the size of the gap with interaction depends on the length of the wire. Increasing the length of the finite wire to 7000 nm, while keeping all the other parameters unchanged, we obtain 0.28 meV. Increasing the magnetic field for the infinite wire with interaction the gap of the BdG spectrum decreases. For example it becomes 0.20 meV for $B_y = 0.37 \text{ T}$ and nearly zero for $B_y = 0.43 \text{ T}$ if $\mu = 9.4 \text{ meV}$ (not shown). The transition can also be approached by changing the Fermi energy, as in figure 5(b), where the gap is 0.08 meV, for $B_y = 0.2 \text{ T}$ and $\mu = 10.6 \text{ meV}$. The transition of the interacting wire occurs at a slightly higher field. This situation is selected to be compared with figure 2(d) which is for a larger field and hence with the interacting system on the other side of the phase boundary, but with the noninteracting one still in the trivial phase.

4.3. $W$ and $\Gamma$ contributions to the BdG spectra

The Coulomb interaction is included in our model such that the BdG spectrum is consistent with the electronic spectrum of the system in the normal state. The normal state corresponds to
Δ = 0, and in this case the BdG spectrum is the same as for the electrons in the normal quantum wire, only shifted by the chemical potential, and replicated for negative energies via particle–hole symmetry, \( \varepsilon \to -\varepsilon \). Indeed this is true without interaction (as shown in figure 4), since the BdG Hamiltonian becomes block-diagonal in the Nambu space. In the presence of the interaction, the BdG Hamiltonian is still diagonal if \( \Delta = 0 \). The reason is that the contribution to the off-diagonal terms \( \Gamma_{q_1 q'_1} \) contains products of \( u \) and \( v \) wave functions, which for \( \Delta = 0 \) describe pure electrons or pure holes, and hence one of them is zero. The numerical calculations are based on iterations with the initial solution corresponding to the noninteracting case, i.e. with \( \Gamma_{q_1 q'_1} = W_{q_1 q'_1} = 0 \), and if \( \Delta = 0 \) then \( \Gamma_{q_1 q'_1} = 0 \) for each iteration. Only the (Nambu-) diagonal Coulomb term \( W_{q_1 q'_1} \) contributes to the spectrum in the normal state with interaction, which corresponds to pure electrons and holes essentially in the Hartree–Fock approximation. \( W_{q_1 q'_1} \) describes the particle–particle or hole–hole repulsion.

The term \( \Gamma_{q_1 q'_1} \) corresponds to the particle–hole interaction and it is in general small for the parameters that we consider in this work. In the spectra shown for the quantum wire of finite length, the contribution of this term is of the order of 10–3 meV and is low and even negligible, relative to the \( W \) term. Because the matrix elements \( \Gamma_{q_1 q'_1} \) depend on the particle–hole mixing, \( u, v \), equation (20), they have peaks for the wave vectors where energy gaps are small. An example is shown in figure 6(a). The net effect of \( \Gamma \) is, however, very small, as shown in this figure for positive energies, where the spectrum with the full interaction included is compared with the spectrum where only the \( W \) term is used. In the same figure, for negative energies, we compare the spectrum with full interaction with the spectrum without interaction (\( u_0 = 0 \)). So in general, in our study the effects of the interaction on the BdG spectrum are mostly determined by particle–particle and hole–hole interactions, and less by particle–hole interactions.

Furthermore, the effects of the Coulomb interaction decrease when the magnetic field increases. This is seen in figure 6(b), for a magnetic field of 2.8 T. The energy spectrum of the normal wire can be easily distinguished as the quasi-parabolic convex bands with the Fermi level at zero energy. In this case all the occupied states have “spin up”, i.e. along the magnetic field (ignoring the tilting effect of the SOI). The Zeeman energy is larger than the orbital energy and thus the first unoccupied band has the same spin-up orientation and the topological phase transition occurs when the band bottom is zero. As long as only spin-up states are occupied the interaction does not affect the spin-up, but only the spin-down, states. To understand that we can simplify the normal wire to a single orbital band \( E_1(k) \) (i.e. \( n_x = 1 \)), neglect the SOI (\( \alpha = 0 \)) and consider \( u_{q_1 q'_1} \) eigenstates of \( \sigma_y \). The interaction term, equation (19), becomes \( W_{q_1 q'_1} = \lambda \sigma_y \omega_{q_1} \omega_{q'_1} \), and the interacting energies are \( E_1(k) = W_{q_1} \pm \delta_{i,j} \). If only spin-up states are occupied then \( W_{q_1} = w_1 \) and the lowest energy is not affected. The argument can be extended for two or more bands (\( n_x > 1 \)) in a straightforward manner. In fact the result is consistent with the Hubbard model used in Ref. [39], because the interaction has no effect on the many-body ground state if only one spin state is occupied.

4.4. The phase diagram

The two models of quantum wire, with finite or infinite length, give us complementary information on the TQPT and on the presence of Majorana states. In a finite wire, the Majorana
modes localized at opposite ends overlap and, as a result, acquire finite energy. This energy vanishes exponentially in the long wire limit. However, it is rather difficult to describe the TQPT, technically a property of a system with $L_y \to \infty$, based on finite wire calculations. Therefore, the phase transitions are described using the infinite wire model and identified by the vanishing of the quasiparticle gap at $k = 0$ [59]. Nonetheless, our numerical calculations show that the boundary between the trivial and topological superconductor phases, when $\mu$ and $B_y$ are varied, is almost the same as for the finite and infinite wires, both with and without the Coulomb interaction, as also indicated by the previous compared examples. To see the effect of the Coulomb interaction on the phase diagram, for a larger set of parameters, we use the infinite quantum wire and define the phase boundaries as the ($E_Z, \mu$) values which minimize the gap of the BdG spectrum at $k = 0$. The results are shown in figure 7, for the noninteracting case and for two different interaction strengths.

The phase boundaries are practically defined by the parameters corresponding to the chemical potential touching the bottom of a confinement-induced band in the normal state spectrum of the quantum wire [59]. For the noninteracting case these boundaries can be approximated by the linear equations

$$\mu = E_{n_0,0} \pm E_Z/2 = 2.35n_x^2 \pm E_Z/2 \text{meV},$$

(22)

where $n_x = 1, 2, …$ is the orbital band index, equation (21). The effect of the Coulomb interaction can be understood in a simple manner, consistent with our mean-field approximation, i.e. neglecting the correlation term $N_0$. Because of the repulsive nature, the interaction has a positive contribution to the energy spectrum of the normal wire, for any given chemical potential and Zeeman energy. With all band bottoms moving up in energy, a positive energy shift is needed for the chemical potential to approach the phase transition. Therefore, for any fixed $E_Z$ (i.e. a fixed magnetic field) all phase boundaries move up on the $\mu$ scale because of the interaction, except when the system is completely spin polarized. In the absence of Coulomb interaction, according to equation (22), this occurs when $E_Z > 2(\mu - E_{10})$. In this case the interaction has no effect on the low-energy states of the BdG Hamiltonian as illustrated in figure 6(b).

Our results are consistent with those of Stoudenmire et al. obtained for a strictly 1D model [39]. In our phase diagram this is the subdomain corresponding to $n_x = 1$, i.e. the bottom-left corner of figure 7(b), or approximately $\mu < 6$, $E_Z < 7 \text{meV}$. As these authors pointed out, within this subdomain the effect of the interaction is to widen the topological phase at a fixed $E_Z$ [39]. This is not generally true when more subbands are involved. As can be seen in figure 7(a), at higher chemical potentials the phase frontiers can shift either to lower or to higher Zeeman fields in the presence of the interaction. The multicritical points, i.e. the intersections of the phase frontiers, always shift to lower Zeeman fields as the bands become higher. The increase of the slope of the phase boundaries can be understood physically as a result of an interaction-induced renormalization of the effective $g$-factor. This renormalization, which is formally due to the off-diagonal spin contributions to $W_{ig}$ in equation (19), depends on the occupancy of the wire, i.e. on the chemical potential.

At low Zeeman energies the phase diagram has another interesting feature. The corners of the phase boundaries split more and more in the higher bands and the minimum Zeeman energy decreases when the interaction strength increases, as illustrated in figure 7(b). Therefore, by measuring the minimum values of the Zeeman field associated with

Figure 7. (a) The phase diagram in Zeeman energy ($E_Z$)—chemical potential ($\mu$) coordinates. The phase frontiers for different interaction strength, $u_0 = 0, 2$ and $4 \text{eV nm}^2$, are shown with different line types. The weak oscillations of the phase boundaries are generated by numerical noise. (b) The corners of the phase frontiers at low Zeeman field are magnified ten times for visibility, while the relative distance between corners is on the original scale. Due to the interaction the minimum Zeeman energy needed for the topological transition decreases when the chemical potential increases.
the low-energy subbands one can experimentally probe the strength of the interaction effects. Note that, in a noninteracting wire, these minimum values are the same for all subbands, $E_{z}^{\text{c(min)}} = 2\Delta$.

5. Conclusions

We have considered corrections to the BdG Hamiltonian due to short-range repulsive interactions between electrons. The short range interaction is justified by the the screening effect of the superconductor. Our approach corresponds to a Hartree–Fock approximation and neglects higher order correlations. As a reality check we mention that a similar approach has been recently used to describe zero-bias anomalies in short quantum wires, which is in good agreement with our experiments [33]. We have calculated the energy states numerically, with an iterative scheme, for finite and infinite models of quantum wires. We have shown that Majorana states are robust to the Coulomb repulsion. For the parameters that we used the interaction effects are dominated by particle–particle and hole–hole interactions described by the $W$ matrix, equation (19). The particle–hole interaction, described by the $\Gamma$ matrix, equation (20), is in general small or negligible. We have built the phase diagram corresponding to topological phases containing Majorana modes using the model of the infinite quantum wire with several bands. The interaction has no effect on the phase frontiers in fully spin polarized states. For the parameters containing Majorana modes with the model of the infinite quantum wire with several bands. The interaction has no effect on the phase frontiers in fully spin polarized states.

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Appendix

Determining the Coulomb coupling constant $u_0$

A formal justification of equation (6) as well as an estimate for the parameter $u_0$ can be obtained in two different, complementary models. First, we consider a model where each electron in the semiconductor wire creates an image charge in the superconductor metal. If $L_z$ is the thickness of the quantum wire ($L_z \ll L_x \ll L_y$), then the distance between the electron and the image charge is of the order of $L_z$. Any other electron will see the original negative charge of the first one in the company of the reflected positive charge. Therefore a model of an effective screened Coulomb potential (energy) can be

$$ u(\mathbf{r} - \mathbf{r}') = \frac{e^2}{\kappa \left| \mathbf{r} - \mathbf{r}' \right| } \frac{1}{\sqrt{\left| \mathbf{r} - \mathbf{r}' \right|^2 + L_z^2}} , \quad (23) $$

where $\kappa$ is the dielectric constant of the semiconductor host. For a small $L_z$, in the spirit of the theory of distributions, this potential is a precursor of a $\delta$-Dirac function, and equation (23) becomes

$$ u(\mathbf{r} - \mathbf{r}') = \frac{e^2}{\kappa} (2\pi \delta) \delta(\mathbf{r} - \mathbf{r}') , \quad (24) $$

the prefactor being calculated by integrating a well behaved function, and hence $u_0 = 2\pi e^2 L_z/\kappa$. In physical terms a small $L_z$ corresponds to a thickness of the quasi-two-dimensional electron gas that is much smaller than the average inter-electronic distance, i.e. $L_z \ll \lambda_F$. For InSb material $\kappa = 18$ and $L_z = 10$ nm one obtains $u_0 = 5$ eV nm$^2$.

In a complementary approach, we assume that the electrons are localized on atomic lattice sites denoted as $i$ or $j$. The repulsive potential is $u_{ij} = V_{ij}\delta_{ij}$, which in the continuous limit becomes $u(r) = V_{ab}\delta (r) \text{ in 3D}$ and $u(r) = V_{ab}\delta (r)$ in 2D. $a$ is the lattice constant which for InSb is 0.65 nm. The energy parameter $V_0$ can be roughly estimated by integrating the Coulomb potential 1/r in 3D on a sphere of radius $a$ and equating the result with $V_0 a^3$, which gives $V_0 = 2\pi e^2/a$. Then the 2D prefactor of the $\delta$ potential, equation (6), is $u_0 = V_{ab} a^2 = 5.9$ eV nm$^2$.

We can refine the lattice method by assuming the electrons described by atomic orbitals with a constant probability density within a sphere of radius $a$, which is 3/4$\pi a^3$. The electric field inside this uniformly charged sphere is $eia^2$, with $0 < r < a$. The energy of a second electron within this sphere is $\Phi(r) = e(3a^2 - r^2)/2a^2$, where we included the energy of the electron to sit in the center of the sphere, i.e. at $r = 0$. The energy of the pair of electrons is found by the 3D integration on a sphere of radius $a(S_3)$,

$$ V_0 = \frac{3}{4\pi a} \int S_3 \Phi(r) \, dr = \frac{6 e^2}{5 a} \approx 2.7 \text{ eV} . $$

The desired 2D parameter is now $u_0 = V_{ab} a^2 = 1.1$ eV nm$^2$.

In conclusion the interaction parameter $u_0$ in equation (6) should be of the order of eV nm$^2$.

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