How robust are Majorana modes in multiband semiconductor wires?

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We study the emergence of Majorana bound states (MBS) in multiband semiconductor wires with Rashba spin-orbit (SO) coupling, proximity coupled to an s-wave superconductor and in the presence of an external magnetic field. We consider long, but finite, multiband wires (namely, quasi-1D wires with dimensions \(L_x \gg L_y\)). Our numerically exact results demonstrate that interband mixing coming from Rashba SO (Rashba mixing) hybridizes Majorana pairs originating from different transversal modes while simultaneously closing the effective gap. Thus, regions were many MBS coexist are effectively trivial owing to Rashba mixing. On the contrary, Majorana physics is robust provided that only one single transversal mode, not necessarily the lowest one, contributes with a Majorana pair. We also find that Majorana physics is fragile with respect to orbital effects induced by any small out-of-plane component of the magnetic field.

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I. INTRODUCTION

Matter and anti-matter are related by a charge conjugation operation whereby matter and anti-matter obey the relativistic Dirac equation with positive and negative energies, respectively.2,3 Ettore Majorana proved that, under some symmetry considerations, the Dirac equation could admit real solutions corresponding to particle-antiparticle pairs made by the same entity, a Majorana fermion.2,3 Majorana fermions were, firstly, proposed in the context of particle physics to describe neutrinos2,3 and more recently the Majorana search has been revived in the condensed matter2,3 and atomic physics24–33 communities. Apart from the fundamental interest of finding Majorana fermions, part of the excitement comes from the non-Abelian braiding statistics of these particles which could be useful for topological quantum computation34.

The most important breakthrough in the condensed matter context originated with the seminal work of Fu and Kane who predicted that Majorana quasi-particles should appear in topological insulators35 which, in proximity to s-wave superconductors, may behave as topological superconductors. Similar ideas using semiconductors with strong spin-orbit (SO) coupling36–38 rapidly appeared. Arguably, the most promising semiconductor proposals are based on semiconductor nanowires (NW) with strong SO and giant Zeeman splittings, like InAs39 and InSb40,41. This, together with the ability to induce superconductivity42–44, has spurred a great deal of experimental activity towards detecting Majoranas in NWs. In one dimension (1D), these systems support a helical liquid state, where and external magnetic field perpendicular to the SO field forces opposite spin states to move in opposite directions45. In the presence of superconducting pairing, such helical state may become a topological superconductor supporting Majorana modes which appear as zero-energy Andreev bound states46–48. It can be shown that this system is equivalent to Kitaev’s model of 1D spinless p-wave superconductors49. Such ideas have been recently generalized to the more realistic case of quasi-1D systems where the effect of transverse modes is taken into account. Both quasi-1D NWs50–57 and p-wave superconductors58,59 have been treated. From these works, an interesting picture emerges of successive filling of subbands giving rise to alternating trivial/non-trivial topological phases. The main idea behind this behaviour is that multiband systems can support 1D topological superconducting phases with MBS provided that there is an odd number of partially occupied bands and that the width of the quasi-1D geometry does not exceed the superconducting coherence length. Note, however, that rigorous topology criteria can only be applied for infinitely long strips where \(Z_2\) invariants, such as the Majorana number39, unambiguously determine the phase diagram. Thus, more finite-system studies beyond effective two-band models41,44 and tight-binding40,42,45 are needed. Relevant questions such as the appearance of fermionic subgap states48 need to be addressed. Finite size calculations fully taking into account the SO interaction are important inasmuch as the creation of long nanowires supporting a single propagating mode is still an experimental challenge.
We here address such task by performing numerically exact diagonalizations of the full SO model of a realistic quasi-1D nanowire in the clean limit. In particular, we study fundamental issues related to the robustness of Majorana physics against (i) spin-orbit interband mixing, (ii) finite size effects, and (iii) magnetic orbital effects. Based on our results we draw two possible favorable scenarios for the experimental detection of Majorana-like states. In the first one, Majorana physics is robust provided that only one single transversal mode, not necessarily the lowest one, contributes with a single Majorana pair. This condition originates from interband Rashba mixing which strongly hybridizes the Majorana modes in situations where more than one pair of them coexist. Alternatively, we show that systems with negligible SO mixing may host many zero energy modes. This second scenario can be achieved in NWs without interband SO interaction. Such situation can be engineered in NWs without SO where either curvature or an inhomogeneous Zeeman field generate an effective band-diagonal SO coupling. We also stress the importance of the orientation of the magnetic field for the Majorana physics detection. Any misalignment of the plane of the NW introduces undesirable magnetic orbital effects that, as shown below, affect dramatically the formation of Majorana modes.

II. QUANTUM WIRE MODELIZATION

We consider a quasi-1D semiconductor strip with a strong Rashba SO and proximity-induced pairing, in the presence of a magnetic field $B$ arbitrarily oriented (see Fig. 1). The model Hamiltonian can be written as $\mathcal{H}_{NW} = \mathcal{H}_{SP} + \mathcal{H}_{Z} + \mathcal{H}_{SO}$, where

$$\mathcal{H}_{SP} = \frac{\Pi_x^2 + \Pi_y^2}{2m^*} - \mu + V(x; L_x) + V(y; L_y),$$

$$\mathcal{H}_{Z} = \frac{1}{2} g_{SM} \mu_B \vec{B} \cdot \vec{\sigma},$$

$$\mathcal{H}_{SO} = \frac{\alpha B}{2} (\vec{\sigma} \times \vec{\pi}) \cdot \vec{E},$$

with $m^*$ the effective mass, $\Pi_x = p_x + (e/c)A_x$ the canonical momentum ($e$ is the electrons charge, and $c$ is the light speed) and $\vec{A}$ the potential vector. $\mathcal{H}_{SP}$ is the single particle energy, refered to the chemical potential $\mu$, in a hard-wall confinement in both $x$ and $y$ directions, given by $V(a; L) = 0$ for $0 < a < L$ and $V(a; L) = \infty$ otherwise. $\mathcal{H}_{Z}$ is the standard Zeeman term, with $\Delta_B \equiv g_{SM} \mu_B B/2$ being the Zeeman energy. $\mathcal{H}_{SO}$ is the Rashba SO Hamiltonian. The constant vector $\vec{E}$ in $\mathcal{H}_{SO}$ corresponds to the effective electric field due to confinement. In our quasi-1D geometry, typical of Rashba systems, the strongest confinement occurs along the $z$ axis and, therefore, $\mathcal{H}_{SO} \approx \alpha (\sigma_y \Pi_z - \sigma_z \Pi_y)$ with $\alpha = \alpha_R E_z/2$. In a convenient gauge, $\vec{A} = -B_z y \hat{u}_z$, it is $\Pi_x = p_x + e y B_z/c$ and $\Pi_y = p_y$. Notice then that both $\mathcal{H}_{SP}$ and $\mathcal{H}_{SO}$ are modified by the magnetic orbital effects, represented by the magnetic length $\ell_z = \sqrt{\hbar c/e B_z}$. More specifically, in the case of the Rashba Hamiltonian we have

$$\mathcal{H}_{SO} = \alpha_x p_x \sigma_y - \alpha_y p_y \sigma_x - \frac{\alpha_e}{\ell_z^2} y \sigma_y,$$

where the distinction between $\alpha_x$ and $\alpha_y$ is artificially introduced. Clearly, in Rashba NWs $\alpha_x = \alpha_y = \alpha$, however in a recent proposal situations with $\alpha_y \neq \alpha_x$, including the case $\alpha_y = 0$, can also be engineered. This is achieved in NWs without SO interaction using inhomogeneous fields $B(x)$ or modulated g-factors $g_{SM}(x)$. In general, Eq. (4) mixes different quantum well subbands in $x$ (through the $p_x$ operator) and in $y$ ($p_y$ and $y$ operators). Assuming the condition $L_x \gg L_y$ the relevant mixing term is $\alpha_y p_y \sigma_x$ that we name Rashba mixing. Finally, we stress that orbital effects modify the SO coupling, including the Rashba mixing, and, as shown below, alter dramatically the topological phases of multiband nanowires. The second-quantized Hamiltonian can be written as $\mathcal{H}_{NW} \rightarrow \sum_{n,n'} \sum_{\sigma,\sigma'} (\sigma \abs{\mathcal{H}_{NW}} \sigma') c_{n \sigma}^\dagger c_{n' \sigma'}$, where $n \equiv \{n_x, n_y\}$ are the quantum numbers associated with the transversal modes due to confinement and $\sigma = \uparrow, \downarrow$ denotes the spin. When the nanowire is proximity-coupled to an ordinary s-wave superconductor we add the BCS-Rashba-BdG Hamiltonian, $\mathcal{H}_{BCS} = \frac{1}{2} \sum_{n,n'} \Psi_n^\dagger \mathcal{H}_{BdG} \Psi_{n'}$, where $\Psi_n = (c_{n \uparrow}, c_{n \downarrow}, c_{n \downarrow}, -c_{n \uparrow})^\dagger$ and

$$\mathcal{H}_{BdG}^{(n,n')} = \frac{\Delta_{\mathcal{H}_{NW}}}{\Delta} \left( \begin{array}{cc} \Delta & i \sigma_y \mathcal{H}_{NW}^{(n)} \sigma_y \\ i \sigma_y \mathcal{H}_{NW}^{(n')} \sigma_y & -\Delta \end{array} \right).$$

Our results below, obtained by exact numerical diagonalization of Eq. (5), demonstrate the emergence of NW gapped low-energy eigenstates; ideally zero modes separated by a sizeable energy gap from the rest of the spectrum and, as anticipated, we will focus on the robustness of this behavior.

III. MAJORANA-LIKE BEHAVIOR IN FINITE NANOWIRES

As good estimates, let us notice that in infinite 1D nanowires the occurrence of a Majorana pair requires large enough Zeeman energies with fields exceeding a critical value $B_c$ given by $g_{SM} \mu_B B_c/2 = \sqrt{\mu^2 + \Delta^2}$. In the quasi-1D case, a similar condition for the critical field $B_c^{(y)}(n_y)$ of the Majorana pair from each $n_y$ transverse mode is $g_{SM} \mu_B B_c^{(y)}(n_y)/2 = \sqrt{(\varepsilon_{n_y} - \mu)^2 + \Delta^2}$, with $\varepsilon_{n_y}$ the transverse mode energy. Our results of Fig. 2, corresponding to the absence of Rashba mixing, confirm this scenario in long-enough wires and for field along $\hat{x}$. We clearly see that increasing the field strength, successive gapped low-energy pairs, each belonging to a different
transverse mode, appear in the spectrum. This picture is consistent with the results of Refs.\textsuperscript{40–42}. We emphasize, however, that Fig. 2 corresponds to a situation in which transverse modes are uncoupled. Moreover, the pair energies are not exactly zero, but oscillate around zero with increasing $B$, showing a steadily increasing amplitude. This is a finite size effect, indicating that the shortness of the wire eventually dominates, removing the pairs from zero energy and destroying the gap with the nearby states as well. The existence of gapped low-energy modes (ideally zero modes) and particle-hole symmetry are the requirements for the emergence of Majorana physics. Let us label positive energy states at a given $B$ in Fig. 2 by an index $I = 1, 2, \ldots$ in increasing energy order. Analogously, negative energy states in decreasing energy order are labelled by $I = -1, -2, \ldots$. According to Dirac, positive-energy states are particle states while negative ones are their conjugated or antiparticle ones. Clearly, when $|E_I|$ is sizeably nonzero $|I|$ and $|-I|$ are different stationary eigenstates of $H$, particle-antiparticle conjugates of each other. Notice now that we may form the two combinations

$$|\gamma^{(I)}_a\rangle = \frac{1}{\sqrt 2}(|I\rangle + |-I\rangle), \quad |\gamma^{(I)}_b\rangle = \frac{i}{\sqrt 2}(|I\rangle - |-I\rangle),$$

with the remarkable property that each of them is its own antiparticle conjugate. These are the Majorana states that, in general, are not Hamiltonian eigenstates. However, a conspicuous exception occurs when $E_I \approx E_{-I} \approx 0$ since then $|\gamma^{(I)}_a\rangle$ and $|\gamma^{(I)}_b\rangle$ are approximate zero eigenstates of $H$, as occurs with $E_{\pm 1}$ when $\Delta_B > 0.5$ meV in Fig. 2. In this case the pair of Majoranas are gap-protected quasi-eigenstates and thus robust and almost stationary in time, what makes them interesting from the applications point of view.\textsuperscript{43}

IV. ROBUSTNESS AGAINST RASHBA MIXING

As we discussed in the previous section, in the absence of Rashba mixing, $\alpha_y$ in Eq. (4), successive gapped low-energy pairs, each belonging to a different transverse mode, appear in the spectrum. As we discuss now, Rashba mixing makes this so-called even-odd behaviour\textsuperscript{40–42} fragile when many transverse modes contribute to Majorana formation in realistic finite samples ($L_x/L_y = 20$ and $L_y \approx 4\nu L \approx 0.4\xi$, with $L = \frac{k_B \mu}{\pi\Delta}$ and $\xi = \frac{\alpha_y B}{2m^*\Delta}$ being the SO length and the superconducting coherence length, respectively). Panels a and b in Fig. 3 summarize the evolution of a representative spectrum when the mixing is gradually introduced. This mechanism leads to an effective coupling between low energy modes, with relevant modifications of the spectra in the regions that for Fig. 2 contained two and three Majoranas. After the collapse of the second mode, a small gap near zero energy appears in Fig. 3b. Moreover, the presence of Rashba mixing tends to close the separation gap between low energy and higher energy states. These effects are thus quenching the robustness of the Majorana modes by making them lose both their zero-energy character and their gap-protection from the rest of the states. Overall, all the regions with more than one Majorana pair, namely $\Delta_B > 0.75$ meV for Fig. 3b, become trivial. The density distributions of the three lowest eigenstates for $\Delta_B = 4$ meV is shown in Fig. 3b, proving that the character of edge modes is lost in presence of full Rashba mixing. On the other hand, the region with one Majorana pair, approximately in the range $0.25$ meV $< \Delta_B < 0.75$ meV in Fig. 3b, is clearly gapped. We have performed detailed calculations as a function of the chemical potential (Appendix) that prove that these regions with a single Majorana pair are robust. Moreover, they show alternating trivial and non-trivial behavior as the chemical potential increases\textsuperscript{40–43,46}. This alternating behavior appears as successive transversal modes are filled and a single Majorana pair, originated from the highest mode, appears. Therefore: 1) Majoranas do not necessarily emerge from the first transverse mode and 2) they are robust even in regions $\mu \gg \Delta_B$, namely in situations where a single band NW would be trivial. Our results place the Rashba mixing as ultimate responsible of the absence of clear
sequences of nontrivial/trivial phases for large magnetic fields. Thus, a good strategy towards detecting Majoranas is to measure at magnetic fields close to the critical field when the first transversal mode contributes with one Majorana pair. In such situation, the successive filling of high transversal modes, as one increases the chemical potential, will produce alternating nontrivial regions with a single Majorana pair each, so that Rashba mixing is not efficient. We emphasize that, for the lengths we have considered, we do not find such alternating behavior between trivial and non-trivial phases by varying the Zeeman field, as opposed to Ref.42. Nevertheless, even-odd physics in the whole $(\mu, \Delta_B)$ phase space should be recovered for long enough samples where topological arguments become exact. We have checked that this is indeed the case by performing Pfaffian calculations (Appendix). Note that, of course, the contrary is not true and Pfaffian calculations, valid when momentum along the wire is a good quantum number, do show non-trivial regions for values of $\mu$ and $\Delta_B$ where the exact calculations for realistic finite-size wires predict trivial behavior.

V. ROBUSTNESS AGAINST ORBITAL EFFECTS

All the above results were obtained assuming a magnetic field with a perfect in-plane orientation. We finish this discussion by studying the role of magnetic orbital effects, due to $B_z \neq 0$. The polar angle $\theta_c = \tan^{-1} B_z/B_x$ quantifies an unwanted small out-of-plane component of the magnetic field. Our results are shown in Fig. 4. A rather small vertical component of the field is sufficient to steadily increase the energy of the lowest mode, from a clear Majorana-like character with $E_1 \approx 0$ for $\theta_c = 0^\circ$ to $E_1 \approx 0.2\Delta$ for $\theta_c = 3^\circ$. At the same time, the gap from the lowest to the next state, $E_2 - E_1$, is reduced as the magnetic field inclination decreases. Thus, orbital
effects severely suppress the Majorana character of the low-energy modes. This is demonstrated in Fig. 4(b), where just one degree of tilting is enough for the spectrum not to show gapped low energy modes as a function of $B$.

VI. CONCLUSIONS

We report the existence of Majorana modes in quasi-1D semiconductor wires. We draw two possible practical scenarios for the detection of this gapped low-energy eigenstates: (i) Rashba NWs hosting a single Majorana pair; (ii) NWs with negligible SO interband mixing which can host many zero energy modes. This second scenario can be engineered in NWs without interband SO interaction. Finally, we have addressed the fragility of the Majorana behavior against magnetic orbital effects, finding that a small misalignment of the magnetic field with respect to the NW is sufficient to quench Majorana physics.

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Appendix A: Supplementary Information

1. Robustness of Majorana-like states against chemical potential

In this appendix we present results for the nanowire spectrum as a function of the chemical potential. These results demonstrate that, in the presence of Rashba mixing ($\alpha_y$Dy$\sigma_x$ term in Eq. 4 of the main text), regions with a single Majorana pair are robust while regions where Majorana pairs coexist are not. To illustrate this, we first show the spectrum without Rashba mixing (Fig. 5, upper panel). This energy spectrum can be understood as a superposition of the partial spectra corresponding to subspaces of the transversal modes $n_y = 1, 2, 3 \cdots$. For low $B$ fields (Fig. 5a for $\Delta_B = 0.48$ meV) single Majorana pairs never coexist: as $\mu$ increases, successive traversal modes $n_y = 1, 2, 3 \cdots$ become populated and contribute with a Majorana mode each. These regions with Majoranas are separated by gapped regions without zero modes. These intermediate regions correspond to solutions with contributions from different $n_y$ (for instance, the region around $\mu = 2.5$ meV corresponds to solutions where both $n_y = 2$ and $n_y = 3$ have a significant weight).

At high magnetic fields (Fig. 5b for $\Delta_B = 2.4$ meV) Majorana-like states from different transversal modes (i.e., different $n_y$) have a substantial overlap. One, two and three Majorana-like states can coexist as shown in Fig. 5b (the region with three Majoranas is distorted because of finite size effects). We emphasize, again, that this coexistence of Majorana modes is possible owing to the absence of SO mixing. As we discuss below, a full calculation (Fig. 5d) shows that these regions are indeed trivial. For low $B$ fields, where only one Majorana pair appears in the spectrum, the physics is similar without or with Rashba mixing (Fig. 5c for $\Delta_B = 0.48$ meV). Namely, alternating trivial/nontrivial regions separated by gapped regions without zero modes. Interestingly, non-trivial regions occur even for large chemical potentials $\mu \gg \Delta_B$ (e.g. the region around $\mu = 3$ meV in Fig. 5c). This result is in agreement with Refs. 42 and 43. However, at high $B$ fields (Fig. 5d for $\Delta_B = 2.4$ meV), the coexistence of various Majorana states is removed because of the Rashba mixing. All modes strongly hybridize, gapped regions disappear and the full spectrum is trivial. We thus conclude that in the presence of Rashba coupling, the only robust Majorana regions are those with single Majorana pairs. Therefore, alternating trivial and non-trivial regions can be expected in situations where only a single Majorana pair exists. Importantly: 1) this Majorana does not necessarily emerge from the first transverse mode and 2) they are robust even in regions $\mu \gg \Delta_B$, namely in situations where a single band nanowire would be trivial. These results support the fact that Rashba mixing is the ultimate responsible of the absence of clear sequences of nontrivial/trivial phases for large magnetic fields.
2. Phase diagram in the $L_x \rightarrow \infty$ limit

Our results are obtained by finite-size numerically exact calculations so it is interesting to investigate to what extent they agree with exact topological phase diagrams in the $L_x \rightarrow \infty$ limit. In order to do so, we have also performed Pfaffian calculations for an infinitely long nanowire (Fig. 6). Using the Pfaffian one predicts alternating trivial/non-trivial regions in the phase space $(\mu, \Delta_B)$. At low fields, this even-odd behavior agrees with our full results where the filling of successive $n_y$ contributing with a Majorana mode each gives robust non-trivial regions, even with SO mixing. At high fields, however, the Pfaffian still shows even-odd behavior in regions where the spectra of our full calculations gives strongly hybridized modes and, hence, trivial behaviour. Thus, Pfaffian calculations seem to become unreliable in regions where many transversal modes contribute with Majoranas and overlap. This can be understood as finite-size effects, very relevant in the case of strong SO mixing, are completely neglected. In such situations, full calculations, as the one presented here, are needed.

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Note also that interband superconducting pairing (not included here) has been shown to induce “sweet spots”, namely ranges of Zeeman coupling for which the system is in the nontrivial phase for any value of $\mu^{41,42}$. 

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