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# Topological phases and transport properties of screened interacting quantum wires

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ABSTRACT

We study theoretically the effects of long-range and on-site Coulomb interactions on the topological phases and transport properties of spin–orbit-coupled quasi-one-dimensional quantum wires imposed on a s-wave superconductor. The distributions of the electrostatic potential and charge density are calculated self-consistently within the Hartree approximation. Due to the finite width of the wires and charge repulsion, the potential and density distribute inhomogeneously in the transverse direction and tend to accumulate along the lateral edges where the hard-wall confinement is assumed. This result has profound effects on the topological phases and the differential conductance of the interacting quantum wires and their hybrid junctions with superconductors. Coulomb interactions renormalize the gate voltage and alter the topological phases strongly by enhancing the topological regimes and producing jagged boundaries. Moreover, the multicritical points connecting different topological phases are modified remarkably in striking contrast to the predictions of the two-band model. We further suggest the possible non-magnetic topological phase transitions manipulated externally with the aid of long-range interactions. Finally, the transport properties of normal–superconductor junctions are further examined, in particular, the impacts of Coulomb interactions on the zero-bias peaks related to the Majorana fermions and near zero-energy peaks.



## 1. Introduction

The existence of Majorana fermions (MFs) as elementary particles has been a myth since the original proposal suggested by E. Majorana in 1937 [1]. In recent years, condensed matter physicists have been searching for the Majorana fermions as quasiparticle excitations in various solid state hybrid structures with vigorous efforts attributed to some alluring and promising theoretical predictions [2–4]. The enthusiasm was further ignited by the relevant experimental realizations in semiconductor quantum wires with strong spin–orbit couplings and proximity-induced s-wave superconductivity by Mourik et al. [5] and other groups subsequently [6–8]. In these experiments, zero-bias conductance peaks have been observed due to perfect Andreev reflection, signaling the presence of Majorana states at the ends of quantum wires. The experimental measurements show that the zero-bias differential conductance evolves into peaks as the system is tuned into the predicted topological regime without taking into account various effects, such as the finite-length, finite temperature, and electron–electron interactions etc. To clarify some discrepancies between experiments and theories, the effects of disorder [9,10], nonclosure of gaps [11], inhomogeneous pairing potentials [12] have been investigated theoretically. More severely, alternative mechanisms, for example, the Andreev bound state [13] and the Kondo effect [14] which also produce the zero-bias peaks have been suggested to challenge the experimental findings.

Among all the aforementioned effects, the electronic interaction is of vital importance and tricky to treat microscopically [15]. It is expected that Coulomb interactions can strongly influence the stability of Majorana modes [16–18], and are, therefore, crucial for understanding quantitatively the experimental findings and ultimately recognition of the existence of Majorana bound states at the ends of quantum wires. In the one-dimensional (1D) quantum wires, repulsive interacting electrons form interacting Luttinger liquids and should be described more precisely by the corresponding theory [19,17]. To attack this problem, various methods have been employed. Based on the density matrix renormalization group (DMRG), tunneling spectra of interacting Kitaev chains and Majorana edge states have been examined [15]. In particular, E. Stoudenmire et al. [20] compared systematically the DMRG, Hartree–Fock, and bosonization approaches for treating the interacting Majorana wires and found that the interaction problem can

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be described reasonably well using Hartree–Fock theory with the sufficiently strong proximity effect and applied magnetic fields albeit it deserves more powerful DMRG and bosonization techniques. Besides the single-mode wires, multichannel wires have also been studied considerably [21–25]. Lutchyn et al. [22] have studied the roles of interactions on the low-energy topological phase diagram near the multicritical point connecting the topological phases originating from the first and second transverse subbands, and revealed that the interactions renormalize the phase boundary near the multicritical point leading to the hybridization of Majorana modes from different subbands. Furthermore, the presence of disorder was found to induce the phase transition from topological phases to trivial localized phases together with interactions [26].

In a realistic experimental setup, the semiconducting quantum wire with a high g-factor and spin–orbit coupling is exposed on a metallic s-wave superconductor to get a proximity energy gap. The metallic superconductor, as a secondary effect, may drive the electronic interactions into a strongly screened regime [27]. Consequently, the electronic density and potential distributions in multiband nanowires are rather inhomogeneous along the transverse direction due to the finite width and electronic repulsions. This inhomogeneity in electrostatic potential can be one of the major sources of the soft superconducting gaps. For the transport properties of the semiconductor–superconductor hybrid structures, much of the prior work has been focusing on the non-interacting cases [28,29,19,30–32]. How the screened interactions and the inhomogeneous potential distribution influence the topological phases in multiband quantum wires and the related Majorana modes, has received relatively less attention. In this work, we study the topological phases and Majorana zero mode in a typical experiment-relevant semiconductor–superconductor hybrid device composed of an interacting quantum wire in proximity to a s-wave superconductor. The screened Coulomb interactions are incorporated by the self-consistent Hartree–Fock calculations in the presence of external magnetic fields. It is shown that electron–electron interactions strongly change the energy bands and modify the topological phase boundaries as well as the emergence of Majorana modes.

The paper is organized as follows. In Sec. 2 we introduce the structure to be investigated and formulate our model. The calculation results are presented and discussed in Sec. 3. Sec. 4 contains the summary and conclusions.

## 2. Theoretical model

We consider a spin–orbit-coupled semiconductor quantum wire of the width $W$ in the $y$-direction and the length $L$ along the $x$-direction deposited on an s-wave superconducting electrode, while its left side is contacted through a tunnel barrier $U_p$ by a normal metallic lead as shown in Fig. 1(a). The s-wave superconductor induces a paring potential $\Delta$ for the electrons in the wire. The whole system is subjected to a uniform in-plane magnetic field $B_x$. Throughout the calculations, we choose the realistic parameters for InSb semiconductor quantum wires: $\Delta = 0.25$ meV, g-factor $g = 50$, Rashba spin–orbit coupling strength $t_R = 20$ meV $\cdot$ nm, and effective mass $m^* = 0.015m_e$ with $m_e$ being the electron mass [5,6,33].

The system is described by the tight-binding Hamiltonian consisting of three terms as

$$\mathcal{H} = H_0 + H_R + H_U, \tag{1}$$

with respective form given by

$$H_0 = \sum_{i,\sigma} c^\dagger_{i,\sigma}(\epsilon_0 + V_H - eV_g)c_{i,\sigma} - t\sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} + \frac{1}{2}g\mu_B\sum_{i;\sigma,\sigma'} c^\dagger_{i,\sigma}s_xB_xc_{i,\sigma'}; \tag{2}$$

$$H_R = it_R\sum_{\langle i,j\rangle;\sigma,\sigma'} \hat{\mathbf{e}}_z\cdot(\mathbf{s}\times\mathbf{d}_{ij})c^\dagger_{i,\sigma}c_{j,\sigma'}; \tag{3}$$

$$H_U = U\sum_{i,\sigma} n_{i\sigma}n_{i\bar{\sigma}}, \tag{4}$$

where $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ are creation and annihilation operators for an electron with spin $\sigma(\uparrow,\downarrow)$ on site $i$, and $\mathbf{s}$ denotes the Pauli matrices. The Hamiltonian $H_0$ in Eq. (2) represents the Hamiltonian of semiconductor quantum wires including the on-site energy $\epsilon_0 = -4t$ and the hopping energy $t$ between the nearest-neighboring sites along $x$- and $y$-directions. $V_H$ and $eV_g$ are the Hartree potential and the potential from gate voltages, respectively. $V_g$ and $e$ are respective the gate voltage and the electron charge. It is the gate voltage that induces extra charges into the wire. Thus, $eV_g$ plays a similar role to the chemical potential in the non-interacting model.

The last contribution is from the Zeeman splitting due to the in-plane magnetic field $B_x$ where magnetic fields only affect the local spins. For high-order effects, the term due to the magnetic field impacts on nonlocal spins might be included. The role of this high-order term will be analogous to that of the spin–orbit coupling and is to decrease the requirement of the spin–orbit strength for topological phases. The term $H_R$ in Eq. (3) describes the Rashba spin–orbit coupling with $\mathbf{d}_{ij}$ being a lattice vector pointing from site $j$ to site $i$. $\langle\rangle$ runs over all the nearest-neighboring sites. The on-site electronic interactions between electrons of the opposite spins are captured by the Hubbard-like term $H_U$ in Eq. (4). To facilitate the computation, Eq. (4) can be rewritten within the mean-field approximation such that a charge with spin $\sigma$ at the site $\mathbf{r}_i$ interacts with the average charge population with an opposite spin $\langle n_{\bar{\sigma}}\rangle$ at the same site and vice versa. The Hubbard-like interaction with different strengths has been treated in various techniques, which suggests that the mean-field approximation is sufficiently exact compared with the DMRG approach provided that the interaction is not very strong [20]. Throughout this work, we use $U = 4\Delta$ which ensures the validity of the mean-field approach. The effects from varying the strength $U$ are not our major purposes since they have been investigated systematically.

Moreover, the Hartree term $V_H(\mathbf{r})$ in Eq. (2) depicts the long-range Coulomb interactions between charges at different sites in the semiconducting quantum wire, [34,27]

$$V_H(\mathbf{r}_i) = \frac{e^2}{4\pi\epsilon_0\epsilon_r}\sum_{\mathbf{r}_i\neq\mathbf{r}_j} n(\mathbf{r}_j)\left(\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} - \frac{1}{\sqrt{|\mathbf{r}_i-\mathbf{r}_j|^2+4d^2}}\right), \tag{5}$$

where $d$ is the distance between the quantum wire and the superconducting metallic gate, and the second part in the parentheses is the contribution from the mirror charges due to the presence of the metallic superconducting gate. It is the solution of the Poisson equation with the present boundary conditions. The mirror charge term screens the Coulomb interactions and reduces the field effects of gates [35]. The average charge population at the site $\mathbf{r}_i$ is calculated by

$$\langle n_\sigma(\mathbf{r}_i)\rangle = -\frac{1}{\pi}\int_{-\infty}^{eV_g} \Im[G_\sigma(\mathbf{r}_i,\mathbf{r}_i;E)]f_{FD}(E,E_F)dE, \tag{6}$$

where $G_\sigma(\mathbf{r}_i,\mathbf{r}_i;E)$ is the Green's function on the site $\mathbf{r}_i$ at energy $E$ for spin $\sigma$. From the computational point of view, both short- or long-range Coulomb interactions affect only the diagonal elements of the Hamiltonian matrix. Eqs. (1)–(6) can be solved self-consistently starting from some initial guess of charge density