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Superconductivity in quantum wires: A symmetry analysis

K.V. Samokhin

Department of Physics, Brock University, St. Catharines, Ontario L2S 3A1, Canada

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ABSTRACT

We study properties of quantum wires with spin–orbit coupling and time reversal symmetry breaking, in normal and superconducting states. Electronic band structures are classified according to quasi-one-dimensional magnetic point groups, or magnetic classes. The latter belong to one of three distinct types, depending on the way the time reversal operation appears in the group elements. The superconducting gap functions are constructed using antiunitary operations and have different symmetry properties depending on the type of the magnetic point group. We obtain the spectrum of the Andreev boundary modes near the end of the wire in a model-independent way, using the semiclassical approach with the boundary conditions described by a phenomenological scattering matrix. Explicit expressions for the bulk topological invariants controlling the number of the boundary zero modes are presented in the general multiband case for two types of the magnetic point groups with real order parameters, corresponding to DIII and BDI symmetry classes.

1. Introduction

Inspired by both the fundamental interest and also potential applications to quantum computing, the search for Majorana fermions (MFs) has become one of the central topics in condensed matter physics, see Refs. [1–4] for reviews. One of the most promising routes to the MFs is based on the observation that a one-dimensional (1D) lattice model of a spin-polarized *p*-wave superconductor, known as the Kitaev chain [5], can have unpaired, or "dangling", zero-energy boundary states near its ends (although these states are not usual fermions, in particular, they have a non-Abelian exchange

E-mail address: kirill.samokhin@brocku.ca.

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statistics, we will still call them MFs, following a considerable precedent in the literature). One can engineer a Kitaev chain-like system in a quantum wire with the spin–orbit coupling (SOC) and a sufficiently strong time reversal (TR) symmetry breaking, in which superconductivity is induced by proximity with a conventional bulk superconductor [6,7]. It is in this setup that experimental signatures consistent with the MFs have been observed, in InSb nanowires in an applied magnetic field [8], and also in ferromagnetic chains on a superconducting Pb substrate [9].

Both crucial ingredients of the recent MF proposals, the asymmetric SOC and TR symmetry breaking, are known to fundamentally affect superconductivity. The asymmetric, or Rashba, SOC (Refs. [10] and [11]) requires the absence of inversion symmetry, which naturally occurs in a quantum wire placed on a substrate. It lifts the spin degeneracy of the electron states, resulting in nondegenerate Bloch bands characterized by a nontrivial momentum-space topology. This has profound consequences for superconductivity in three-dimensional (3D) and two-dimensional (2D) materials, which have been extensively studied in the last decade, see Refs. [12] and [13] for reviews. On the other hand, a TR symmetry-breaking field, either intrinsic (*e.g.*, the exchange field in ferromagnets) or externally applied, also lifts the spin degeneracy of the bands and significantly changes the symmetry properties of the Cooper pairs [14,15].

The first goal of this work is to present a complete symmetry-based analysis of the electronic bands and the superconducting states in the presence of *both* the asymmetric SOC and a TR symmetry-breaking field. Regardless of the microscopic mechanism of pairing, the symmetry approach has proven to be an extremely powerful tool in the studies of unconventional superconductivity, helping to identify possible stable states and determine the gap structure [16]. We focus on the quasi-1D case and develop our analysis without any model-specific assumptions, for an arbitrary number of bands. We emphasize, in particular, the crucial role of antiunitary symmetries in defining the proper gap function.

Our second goal is to calculate the spectrum of the subgap Andreev bound states (ABS) near the ends of superconducting quantum wires, again in a model-independent way. The presence of these states, observed, *e.g.*, in high-T_c cuprates and other materials [17], is an important signature of an unconventional pairing. The ABS energies are obtained by solving the Bogoliubov–de Gennes (BdG) equations in the semiclassical, or Andreev, approximation [18]. The MFs emerge as zero-energy ABS protected by topology against sufficiently small perturbations. According to the bulk-boundary correspondence principle, the number of the boundary zero modes is determined by a certain topological invariant in the bulk [19,20]. We prove this statement in the systems under consideration and present explicit expressions for the number of zero modes for different types of the magnetic classes.

The rest of the paper is organized as follows. In Sections 2 and 3, we introduce the 1D magnetic points groups, or magnetic classes, and develop a symmetry classification of quasi-1D electron band structures. In Section 4, superconducting pairing is analyzed for different types of the magnetic classes. In Section 5, we use the semiclassical approach to calculate the ABS spectrum in a general multiband quasi-1D superconductor, in particular, to count the number of zero-energy modes protected against symmetry-preserving perturbations. Section 6 contains a summary of our results. Throughout the paper we use the units in which $\hbar = 1$, neglecting the difference between the quasiparticle momentum and wavevector, and denote the absolute value of the electron charge by e.

2. Magnetic classes in one dimension

We consider a quasi-1D wire oriented along the x direction on a xy-plane substrate. The full 3D potential energy $U(x, y, z)$ affecting the electrons is periodic in x, with the period d, but confining in both y and z directions. This system lacks an inversion center, because the substrate breaks the $z \to -z$ mirror reflection symmetry. In the presence of a uniform external magnetic field $\boldsymbol{H} = \nabla \times \boldsymbol{A}$, the single-particle Hamiltonian has the following form:

$$\hat{H} = \frac{\hat{\boldsymbol{P}}^2}{2m} + U(\boldsymbol{r}) + \frac{1}{4m^2c^2}\hat{\boldsymbol{\sigma}}[\nabla U(\boldsymbol{r}) \times \hat{\boldsymbol{P}}] + \mu_B\hat{\boldsymbol{\sigma}}\boldsymbol{H}. \tag{1}$$

Here $\hat{\boldsymbol{P}} = \hat{\boldsymbol{p}} + (e/c)\boldsymbol{A}(\boldsymbol{r})$ and $\hat{\boldsymbol{p}} = -i\nabla$ are the kinetic and canonical momenta operators, respectively, $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$ are the Pauli matrices, and μ_B is the Bohr magneton. The third term describes the SOC