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Synergy of Semiconductor Physics and Electron Pairing: Route Towards Novel Topological Materials

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We discuss possible scenarios for the realization of a topologically nontrivial superconducting phase in the heterostructures composed of semiconducting nanowires proximitized to bulk superconductors. The investigated samples are characterized by Majorana-type modes appearing at the boundaries of nanowires. Specifically, we inspect the hypothetical transition to the topological superconducting state of the Rashba nanowire deposited along the crystallographic axis of the CuO_2 plane of a d-wave high T_c superconductor. Such a transition might enable access to the topological phase at much higher temperatures than those experimentally observed so far.

topics: topological superconductivity, Majorana bound states, semiconducting nanowires

1. Introduction

Electrons moving in the crystal lattice are described by Bloch waves, which imply an electron spectrum consisting of energy bands separated by forbidden regions (energy gaps). Intrinsic semiconductors happen to have their Fermi level located inside one of such gaps (width $E_g \simeq$ 1–3 eV) between the filled (valence) and empty (conduction) bands. Since the population of thermally excited charge carriers depends exponentially on the energy gap, i.e., $\mathrm{e}^{-E_g/(k_\mathrm{B}T)}$, therefore at low temperatures T such materials are practically insulating. Upon introducing adatoms with energy levels either near the upper edge of the valence band or the bottom edge of the conduction band, the number of charge carriers is substantially increased. This donor/acceptor doping mechanism has led to the development of modern technology based on semiconducting materials.

A similar picture is realized to some extent also in superconductors, where the formation of electron pairs depletes the single-particle states over a narrow region (of width $\Delta \sim$ meV) around the Fermi energy. Numerous experiments have established that magnetic impurities usually break Cooper pairs, therefore their influence on superconducting materials is detrimental. One can, however, inspect the influence of Cooper pairs back on those impurities whose spectra are observable by tunneling spectroscopy. It turned out that such impurities acquire pairing and are converted into superconducting grains with bound states induced inside the energy window $\langle -\Delta; \Delta \rangle$. These bound states always appear in pairs symmetrically around the Fermi level [1].

Figure 1 displays a comparison of the in-gap states induced by impurities in semiconductors and superconductors. Doped semiconductors are characterized by an additional energy level through which electrons/holes contribute to the conduction/valence band. Doping moves the Fermi level E_F close to the lower/upper edge of the band, increasing the number of charge carriers. In contrast, the impurities introduced to the bulk of the superconductor develop a pair of the bound states at $\pm E_A$ centrally located around E_F. In that case, the Fermi level is pinned in the middle of the pairing gap. The evolution of the in-gap state of a quantum spin Hall insulator into the pair of bound states of a proximity-induced superconductor has been discussed by one of the Authors in [2]. These bound states, known as Andreev quasiparticles or Yu–Shiba–Rusinov quasiparticles, have been the subject of intensive studies because, under specific conditions, they give rise to the topological superconducting phase [3–5].

2. Topological superconductivity

The gaped electronic spectrum of semiconductors (insulators) and superconductors can be useful for obtaining protected boundary modes originating purely from a topological nature. The topology

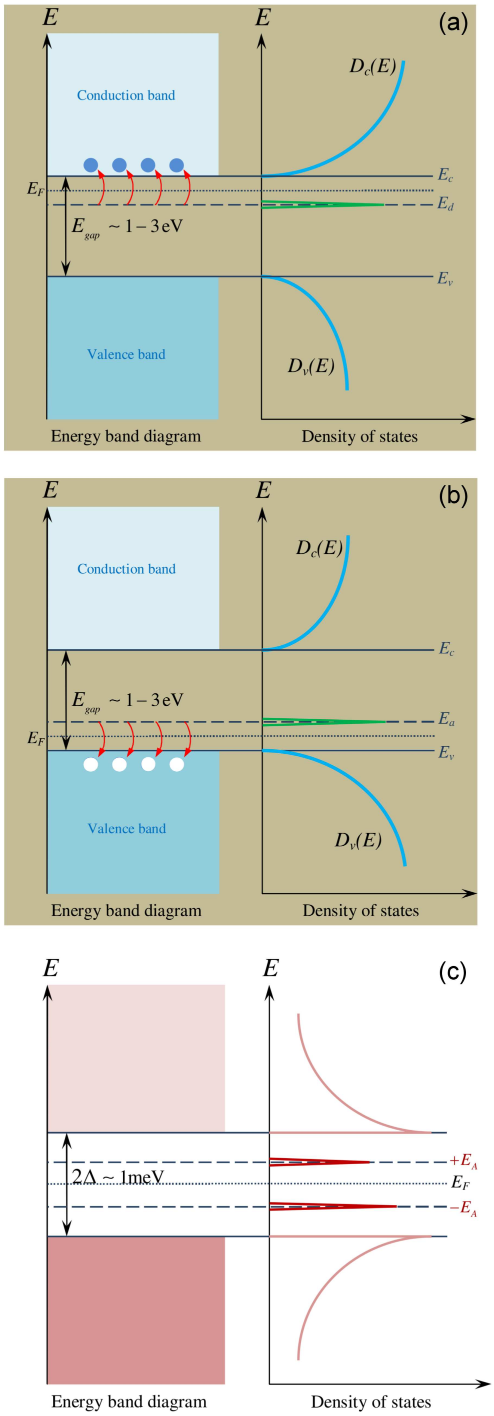

Fig. 1. In-gap states induced by donor/acceptor atoms in semiconductors (panel (a)/(b)) and by impurities in superconductors (panel (c)). The dotted line shows the Fermi level, which is located inside the energy gap in all cases.

of electronic systems is related to the intrinsic geometry implied (by Bloch's theorem) on the manifold of the Brillouin zone. Topological insulators and superconductors [6] are distinct from their ordinary counterparts by characteristic invariants and are classified according to the time-reversal, particle–hole, and chiral symmetries [7]. In one-dimensional systems, these topological invariants are strictly related (via *bulk-boundary correspondence*) to the number of pairs of protected modes appearing at boundaries or internal defects. Specifically, the subgap bound states of magnetic impurities arranged into chains or islands coupled to superconducting bulk materials can undergo a topological transition, developing zero-energy boundary quasiparticles [3–5]. They are reminiscent of Majorana fermions originally proposed in high-energy physics. Such exotic quasiparticles are promising candidates for stable qubits and could be used for quantum computing by virtue of their non-Abelian statistics.

So far, experimental efforts to realize these quasiparticles were mainly focused on one-dimensional structures, such as semiconducting nanowires proximitized to conventional superconductors [8–12], chains of self-organized magnetic atoms deposited on superconducting substrates [13–18], or lithographically fabricated nanostructures covered by superconductors [19]. Topological superconductivity has also been realized in two-dimensional systems, where Majorana quasiparticles acquire a chiral character [2, 20–22].

Another convenient platform for realizing Majorana modes relies on Josephson junctions using narrow metallic strips (with strong spin–orbit coupling) sandwiched between external superconductors [23, 24]. Experimental evidence for the zero-energy modes has been found in such heterostructures, which consist of aluminum on indium arsenide [25] and HgTe quantum well coupled to a thin aluminum film [26]. The topologically non-trivial regime can be easily controlled in such a geometry by the phase difference imposed between the external superconducting leads. It has been suggested that more complex combinations, comprising three superconducting regions interconnected by normal strips, might induce topological superconductivity entirely via the phase control, without any need for Rashba interactions [27, 28]. These recent proposals aim to completely eliminate the magnetic field, the influence of which on superconducting substrates is detrimental.

3. Topological phase of *d*-wave host

Here we propose another realm to access the topological superconducting phase at relatively higher temperatures, using semiconducting nanowires deposited on cuprate superconductors. These materials are characterized by inter-site pairing with the *d*-wave symmetry order parameter. We assume that the semiconducting nanowire is placed along the crystallographic axis of the CuO_2 plane of such high T_c superconductors (see Fig. 2).

A similar proposal of a semiconducting nanowire coupled to mixed (*d*-wave and *s*-wave) symmetry order parameters was considered previously in [29, 30]. In this paper, we focus on the pure

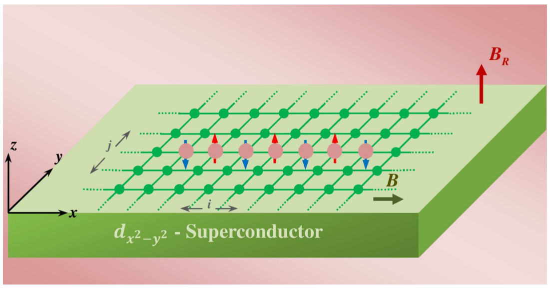

Fig. 2. Schematic view of a semiconducting nanowire deposited on the surface of CuO_2 plane of a high temperature superconductor with proximity-induced singlet pairing. The topological phase can emerge in the presence of the magnetic field B and the spin–orbit Rashba interaction B_R, aligned as indicated.

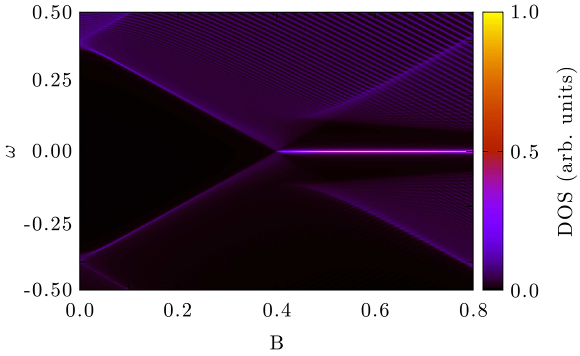

Fig. 3. Transition to the topological superconducting phase of a Rashba nanowire placed in a magnetic field along the crystallographic axis of the CuO_2 plane of the d-wave cuprate superconductor. The results are obtained for the set of model parameters $\mu = -2t$, $\Delta = 0.2t$, $B_R = 0.15t$ of the nanowire consisting of 250 sites.

d-wave superconducting substrate, where the proximity effect spreads the inter-site pairing of electrons in the nanowire. Then, the effective Hamiltonian can be described as follows

$$\hat{\mathcal{H}}^{\rm prox}_{\rm chain} = \sum_{i,j,\sigma} \Big(t_{ij} - \delta_{ij}\, \mu \Big) \hat{d}^\dagger_{i,\sigma} \hat{d}_{j,\sigma} + \Delta \sum_i \Big(\hat{d}^\dagger_{i,\uparrow} \hat{d}^\dagger_{i+1,\downarrow} - \hat{d}^\dagger_{i,\downarrow} \hat{d}^\dagger_{i+1,\uparrow} + {\rm h.c.} \Big) + \hat{\mathcal{H}}_{\rm Rashba} + \hat{\mathcal{H}}_{\rm Zeeman}. \tag{1}$$

The operator $\hat{d}^{(\dagger)}_{i,\sigma}$ annihilates (creates) an electron of spin σ with energy ε_i at the i-th site, t_{ij} is the hopping integral, μ is the chemical potential, and Δ denotes the proximity-induced inter-site singlet pairing. The Rashba interaction

$$\hat{\mathcal{H}}_{\rm Rashba} = -B_{\rm R} \sum_{i,\sigma,\sigma'} \Big[\hat{d}^\dagger_{i+1,\sigma} \left({\rm i}\sigma^y \right)_{\sigma\sigma'} \hat{d}_{i,\sigma'} + {\rm h.c.} \Big] \tag{2}$$

and the Zeeman term

$$\hat{\mathcal{H}}_{\rm Zeeman} = \frac{g\mu_{\rm B} B}{2} \sum_{i,\sigma,\sigma'} \hat{d}^\dagger_{i,\sigma} \left(\sigma^z \right)_{\sigma\sigma'} \hat{d}_{i,\sigma'} \tag{3}$$

are responsible for inducing triplet (p-wave) pairing. In the absence of electron pairing (i.e., for $\Delta = 0$), the Rashba interaction (2) detunes bare electronic dispersion curves of different spin orientations. The Zeeman term (3), on the other hand, opens gaps at the intersections of these spin-dependent dispersion curves. Finally, the superconducting proximity effect can cause the inversion of the band-structure, inducing a transition to topologically nontrivial phase.

For a specific illustration of this mechanism, we diagonalize the model Hamiltonian (1) of our setup by the canonical transformation [1]

$$\hat{d}_{i\uparrow} = \sum_n \left(u_{in\uparrow} \hat{\gamma}_n + v^*_{in\downarrow} \hat{\gamma}^\dagger_n \right), \tag{4}$$

$$\hat{d}^\dagger_{i\downarrow} = \sum_n \left(-v_{in\uparrow} \hat{\gamma}_n + u^*_{in\downarrow} \hat{\gamma}^\dagger_n \right), \tag{5}$$

where $\hat{\gamma}_n$ and $\hat{\gamma}^\dagger_n$ denote the Bogoliubov quasiparticle operators with the corresponding complex coefficients $u_{in\sigma}$ and $v_{in\sigma}$. Their values and the set of eigenergies $\mathcal{E}_n$ were determined by solving the Bogoliubov–de Gennes (BdG) equations

$$\mathcal{E}_n \begin{pmatrix} u_{in\uparrow} \\ v_{in\downarrow} \\ u_{in\downarrow} \\ v_{in\uparrow} \end{pmatrix} = \sum_j \begin{pmatrix} H_{ij\uparrow} & D_{ij} & S^{\uparrow\downarrow}_{ij} & 0 \\ D^*_{ij} & -H^*_{ij\downarrow} & 0 & S^{\downarrow\uparrow}_{ij} \\ S^{\downarrow\uparrow}_{ij} & 0 & H_{ij\downarrow} & D_{ij} \\ 0 & S^{\uparrow\downarrow}_{ij} & D^*_{ij} & -H^*_{ij\uparrow} \end{pmatrix} \begin{pmatrix} u_{jn\uparrow} \\ v_{jn\downarrow} \\ u_{jn\downarrow} \\ v_{jn\uparrow} \end{pmatrix}. \tag{6}$$

The matrix element $H_{ij\sigma} = -t\,\delta_{\langle i,j \rangle} - (\mu + \sigma h)\,\delta_{ij}$ refers to the single-particle part of (1) combined with the Zeeman term (3), $D_{ij} = \Delta\,\delta_{j,i+1}$ denotes the inter-site pairing, and $S^{\sigma\sigma'}_{ij} = -{\rm i}\,\lambda(\sigma_y)_{\sigma\sigma'}\delta_{\langle i,j \rangle}$ accounts for the spin–orbit interaction that mixes electrons of opposite spins, where $S^{\downarrow\uparrow}_{ij} = (S^{\uparrow\downarrow}_{ji})^*$, $S^{\uparrow\uparrow}_{ji} = 0 = S^{\downarrow\downarrow}_{ij}$. Here $\delta_{\langle i,j \rangle}$ is 1 for the neighbouring sites and 0 otherwise.

Figure 3 shows the influence of the magnetic field B on the local density of states (DOS) of the nanowire $\rho(\omega) = \sum_{i,n\sigma} |u_{in\sigma}|^2\,\delta(\omega - \mathcal{E}_n) + |v_{in\sigma}|^2\,\delta(\omega + \mathcal{E}_n)$. Upon approaching the critical value $B = 0.4$ (in the units of $g\mu_{\rm B}/2$), the energy gap closes, and next, at stronger magnetic fields, it reopens. Simultaneously, one pair of finite energy in-gap states merges into the zero-energy mode. Inspecting the spatial profile of these Majorana quasiparticles, we found that they exist in a few peripheral sites of the nanowire, which is in close analogy to previously reported results for such systems on the s-wave superconducting substrates [31, 32].

4. Conclusions

We discussed the in-gap states introduced by impurities, both in semiconducting and superconducting materials. We pointed out that the robust (boundary) in-gap states can originate purely from the topology of the Brillouin zone, imposed by the Bloch character of electrons in periodic lattices. Furthermore, we have presented a brief survey of recent intensive studies that have provided evidence for the topological superconducting state of hybrid structures comprising semiconducting nanowires coupled to superconducting materials. These structures revealed the Majorana zero-energy in-gap modes at the boundaries of proximitized nanoscopic samples. Such exotic quasiparticles have so far been observed at low temperatures (of a few Kelvin or less) using conventional isotropic s-wave superconductors.

Finally, we proposed to consider a Rashba nanowire deposited on the surface of the CuO_2 plane of high T_c superconductors, along the main crystallographic axis (Fig. 2). We have shown that transition to a topologically nontrivial state should be feasible in very much the same fashion as for conventional isotropic superconductors [5]. The main virtue of this proposal would be (i) a relatively higher temperature and (ii) a larger pairing gap, allowing for topologically-protected Majorana modes to emerge. We hope that such a proposal can be verified experimentally.

Acknowledgments

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