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Existence of Majorana bound states near impurities in the case of a small superconducting gap

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ABSTRACT

We consider the edge states of a 2D topological insulator in the presence of the Zeeman field and in proximity to a *s*-wave superconductor. We analytically show that two linearly independent Majorana bound states (MBSs) can appear near the impurity located in a small region in which both the pairing parameter Δ and the Zeeman field *M* may be changed. We find two conditions for the existence of the MBSs: firstly, $|\Delta| \approx |M|$, ie, the superconducting gap in the spectrum should be sufficiently small; secondly, the absolute value of the average *w* of the impurity potential should have a certain value; the last condition is necessary. The equation $|\Delta| = |M|$ determines the boundary of the topological phase of the system, thus the system as a whole must be close to this boundary in relation to the parameters. If the same is true for the impurity region, then the second condition has the form $w \approx \pm v/2$ where *v* is the edge states velocity. In this case, the electron transmission probability is equal to 1 for energies close to zero.

1. Introduction

In condensed matter, the Majorana bound states (MBSs) can be thought of as the zero-energy many-electron excitations; they are quasiparticles with no distinction between particles and antiparticles [1,2]. The MBSs may arise near domain walls between different topological phases in the so-called topological superconductors, in particular, at the ends of the quantum wire, proximity coupled to a superconductor [1-7]. This states are topologically protected, hence they are robust against extrinsic perturbations [2,5-7]. The MBSs may have good prospects of applications in quantum computing [1,5,6]. In theory, their existence is not in doubt, but their experimental observation is still being questioned [1,6].

In this paper we deal with the edge states of a 2D topological insulator in the presence of the Zeeman field and in proximity to a swave superconductor [1,2,5–7]. We will explore the possibility of the existence of MBSs near the impurity located in a small region in which both the pairing parameter Δ and the Zeeman field *M* may change. (See in [8,9] the general discussion on the existence of impurity-induced bound states near zero energy in 1D structures, proximity coupled to a superconductor). Using the Green function of the mean field Bogoliubov-de Gennes Hamiltonian (which we find explicitly), we analytically have proved that two linearly independent MBSs localized at the impurity can arise, but only if $|\Delta| \approx |M|$, ie, for a small superconducting gap in the spectrum, and, in addition, the absolute value of the average *w* of the impurity potential must have a certain value (see below; the latter condition is necessary). We also obtain the explicit expressions for the wave functions of the MBSs. The equation $|\Delta| = |M|$ determines the boundary of the topological phase of our system [4], thus the system as a whole must be close to this boundary in relation to the parameters. If the same is also true for the impurity region, then w should be close to $\pm v/2$ where v is the edge states velocity. In this case the electron transmission probability is equal to 1 for energies close to zero, but outside the gap (cf. the existence of the zero energy conductance peak [3]). Another possibility is discussed in Section 3. The results may be useful for the experimental observation of the MBSs.

2. Spectrum and green function

In this section, we study the following Bogoliubov-de Gennes Hamiltonian [1,2,4,10]:

$$H = \begin{pmatrix} -iv\sigma_x \partial_x + M\sigma_z & \Delta i\sigma_y \\ -\Delta i\sigma_y & iv\sigma_x \partial_x - M\sigma_z \end{pmatrix}$$

where σ_x , σ_y , and σ_z are the Pauli matrices acting in the spin space, the pairing amplitude $\Delta \neq 0$ is assumed to be real, and M = const. Further, we set v=1. The wave functions of the Hamiltonian H have the form

$$\psi = (\psi_1^{\dagger}, \psi_1^{\downarrow}, \psi_2^{\downarrow}, \psi_2^{\downarrow}) = (\psi_1, \psi_1^{\prime}, \psi_2, \psi_2^{\prime})$$

.

Here the components with index 1 and 2 refer to particles and holes,

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respectively.

To investigate the Majorana states and their influence on the scattering pattern, we will use the Green function of the Hamiltonian *H*. We will find this function by solving the equation $(H - E)\psi = \varphi$ or, in more detail,

$$-i\partial_x \psi'_1 - (E - M)\psi_1 + \Delta \psi'_2 = \varphi_1,$$
(1)

$$\begin{split} -i\partial_{x}\psi_{1} &- (E+M)\psi_{1}' - \Delta\psi_{2} = \varphi_{1}', \\ i\partial_{x}\psi_{2}' &- (E+M)\psi_{2} - \Delta\psi_{1}' = \varphi_{2}, \\ i\partial_{x}\psi_{2} &- (E-M)\psi_{2}' + \Delta\psi_{1} = \varphi_{2}', \end{split}$$

with respect to ψ . After Fourier transformation

$$\psi(x) \mapsto \widehat{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ipx} \psi(x) dx$$

we obtain from (1)

$$\begin{pmatrix} -(E-M) & p & 0 & \Delta \\ p & -(E+M) & -\Delta & 0 \\ 0 & -\Delta & -(E+M) & -p \\ \Delta & 0 & -p & -(E-M) \end{pmatrix} \begin{pmatrix} \widehat{\psi}_1 \\ \widehat{\psi}'_1 \\ \widehat{\psi}_2 \\ \widehat{\psi}'_2 \end{pmatrix} = \begin{pmatrix} \widehat{\varphi}_1 \\ \widehat{\varphi}'_1 \\ \widehat{\varphi}_2 \\ \widehat{\varphi}'_2 \end{pmatrix}.$$
(2)

We denote by d = d(p) the determinant of the system (2). Then

$$d = E^{4} - 2E^{2}(M^{2} + p^{2} + \Delta^{2}) + (M^{2} + p^{2} - \Delta^{2})^{2}$$

= $p^{4} - 2p^{2}(E^{2} - M^{2} + \Delta^{2}) + (E^{2} - M^{2} - \Delta^{2})^{2} - 4M^{2}\Delta^{2}.$ (3)

By (3), the equation d=0 is equivalent to the equations $E^2 = (\Delta \pm \sqrt{M^2 + p^2})^2$. Hence the spectrum of *H* is the union of $(-\infty, -\alpha]$ and $[\alpha, \infty)$ where $\alpha = \min\{|M - \Delta|, |M + \Delta|\}$. Also from (3) we have

$$\frac{1}{d} = \frac{1}{(p^2 - p_1^2)(p^2 - p_2^2)} = \frac{1}{p_1^2 - p_2^2} \left(\frac{1}{p^2 - p_1^2} - \frac{1}{p^2 - p_2^2} \right),$$
(4)

 $p_1^2 - p_2^2 = 4E\Delta$

where

$$p_1 = \pm \sqrt{(E+\Delta)^2 - M^2}, p_2 = \pm \sqrt{(E-\Delta)^2 - M^2}.$$
 (5)

First, performing the calculations like [11], we find from (2) and Cramer's rule the Green function of H in the momentum representation and then, using (4) and the known formulas

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{ipx}\widehat{\varphi}(p)dp}{p^2 - a^2} = -\frac{1}{2ia} \int_{-\infty}^{\infty} e^{ia|x-x'|}\varphi(x')dx',$$
$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{ipx}p\widehat{\varphi}(p)dp}{p^2 - a^2} = -\frac{1}{2i} \int_{-\infty}^{\infty} e^{ia|x-x'|} \operatorname{sgn}(x - x')\varphi(x')dx',$$

we obtain it in the coordinate representation. As a result, we get the following expressions:

$$\begin{split} \psi_{1}(x) &= ((H-E)^{-1}\varphi)_{1}(x) = -\frac{E+M}{2ip_{1}} \int_{-\infty}^{\infty} e^{ip_{1}|x-x^{\prime}|}\varphi_{1}(x^{\prime})dx^{\prime} \\ &\quad -\frac{1}{2i} \int_{-\infty}^{\infty} e^{ip_{1}|x-x^{\prime}|}\operatorname{sgn}(x-x^{\prime})\varphi^{\prime}_{1}(x^{\prime})dx^{\prime} \\ &\quad +\frac{A}{2ip_{1}} \int_{-\infty}^{\infty} e^{ip_{1}|x-x^{\prime}|}\varphi^{\prime}_{2}(x^{\prime})dx^{\prime} \\ &\quad +\frac{E+M-\Delta}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x^{\prime}|}p_{1}-e^{ip_{2}|x-x^{\prime}|}p_{2})\varphi_{1}(x^{\prime})dx^{\prime} \\ &\quad +\frac{1}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x^{\prime}|}-e^{ip_{2}|x-x^{\prime}|})\operatorname{sgn}(x-x^{\prime})\varphi^{\prime}_{1}(x^{\prime})dx^{\prime} \end{split}$$
(6)

$$\begin{aligned} -\frac{1}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|} - e^{ip_{2}|x-x'|}) \operatorname{sgn}(x - x')\varphi_{2}(x')dx' \\ + \frac{E + M - \Delta}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|}/p_{1} - e^{ip_{2}|x-x'|}/p_{2})\varphi'_{2}(x')dx', \\ \psi'_{1}(x) &= ((H - E)^{-1}\varphi)'_{1}(x) \\ &= -\frac{E - M}{2ip_{1}} \int_{-\infty}^{\infty} e^{ip_{1}|x-x'|}\varphi'_{1}(x')dx' \\ &- \frac{1}{2i} \int_{-\infty}^{\infty} e^{ip_{1}|x-x'|} \operatorname{sgn}(x - x')\varphi_{1}(x')dx' \\ &- \frac{\Delta}{2ip_{1}} \int_{-\infty}^{\infty} e^{ip_{1}|x-x'|}\varphi_{2}(x')dx' \\ &+ \frac{E - M - \Delta}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|}/p_{1}) \\ &- e^{ip_{2}|x-x'|}/p_{2})\varphi'_{1}(x')dx' \\ &+ \frac{1}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|} - e^{ip_{2}|x-x'|})\operatorname{sgn}(x - x')\varphi_{1}(x')dx' \\ &+ \frac{1}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|} - e^{ip_{2}|x-x'|})\operatorname{sgn}(x - x')\varphi'_{2}(x')dx' \\ &+ \frac{-E + M + \Delta}{4i} \int_{-\infty}^{\infty} (e^{ip_{1}|x-x'|} - e^{ip_{2}|x-x'|})\operatorname{sgn}(x - x')\varphi'_{2}(x')dx' \end{aligned}$$
(7)

another two equations are obtained from (6), (7) by replacing

$$\psi_1 \to -\psi'_2, \, \psi'_1 \to \psi_2, \, \varphi_1 \to -\varphi'_2, \, \varphi'_1 \to \varphi_2, \, \varphi_2 \to \varphi'_1, \, \varphi'_2 \to -\varphi_1.$$

For E not belonging to the spectrum, the signs in (5) are determined by the decrease of the exponential functions. If E belongs to the spectrum, these signs determine the direction of movement of the particles.

3. Results and discussion

3.1. Majorana states

According to [8], the nonmagnetic impurities may lead to subgap bound states in wires only in the presence of a combination of Zeeman splitting and Rashba spin-orbit coupling, which are also required to realize a topological superconducting phase. In our case, the role of the Rashba interaction plays the 1D Dirac Hamiltonian. (Note that it can be directly checked that for $-d^2/dx^2$ instead of the Dirac Hamiltonian, the MBSs do not arise near the impurity).

Let us write the equation describing the eigenfunctions of the Hamiltonian H + V where V is the potential, corresponding to the energy E,

$$\psi = -(H - E)^{-1}V\psi. \tag{8}$$

We use the short-range potential of the form

$$V = \begin{pmatrix} \lambda M + V_0 & 0 & 0 & -\nu \Delta \\ 0 & -\lambda M + V_0 & \nu \Delta & 0 \\ 0 & \nu \Delta & -\lambda M - V_0 & 0 \\ -\nu \Delta & 0 & 0 & \lambda M - V_0 \end{pmatrix} \delta(x)$$
(9)

where λ , ν , and V_0 are arbitrary real constants, modeling the change of the Zeeman field and the pairing parameter and also the presence of the impurity near x = 0. We note that $w = 4V_0$ is the average of the impurity potential (for $\lambda = \nu = 0$). In the results obtained below, we can replace $\delta(x)$ with smooth non-negative even function with a support in a sufficiently small neighborhood of zero, the integral of which is equal to 1. Next, we consider only the even smooth approximation of the Dirac function $\delta(x)$, which corresponds to the symmetrical distribution of values of *V* around zero.

To find the MBSs, we set E=0 in (8), and therefore in the expressions for the Green function (see (6), (7) and the remark after (7)). Then, by (5), $p_1 = p_2 = p = \pm \sqrt{\Delta^2 - M^2}$. To obtain the decrease of the eigenfunctions at infinity, we have to assume that $|M| > |\Delta|$ (see [8] where the authors show the necessity of this condition for the existence

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