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BEHAVIOR OF ANDREEV STATES FOR TOPOLOGICAL PHASE TRANSITION

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We consider three one-dimensional superconducting structures: 1) *the one with p-wave superconductivity*; 2) *the main experimental model of a nanowire with s-wave superconductivity generated by the bulk superconductor due to the proximity effect in an external magnetic field and Rashba spin–orbit interaction*; 3) *the boundary of a two-dimensional topological insulator with an s-wave superconducting order in an external magnetic field. We obtain precise analytic results for the "superconductor–magnetic impurity–superconductor" model. Using the Bogoliubov–de Gennes Hamiltonian, we study the behavior of stable states arising in these structures, with energies near the edges of the energy gap of "electron"* ("*hole*") *type for the first model and "electron plus hole" type for the other two models in the case where the system passes from the topological phase to the trivial one. For the topological phase transition, resonance* (*decaying*) *states turn out to play a major role*; *the spin flip and the change of sign of the charge occur due to the transition of bound states to resonance ones and vice versa with their energy changing to the opposite ones as the gap closes. The results are consistent with the absence of a zero-bias conductance peak in the trivial topological phase observed in a recent experiment.*

Keywords: Bogoliubov–de Gennes Hamiltonian, superconducting gap, Andreev bound state, Majorana bound state, resonance state

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1. Introduction

Majorana bound states (MBSs) arising in "superconductor–normal metal" (SN) or "superconductor–normal metal–superconductor" (SNS) heterostructures on the boundary of a superconductor in the topological phase [1]–[5] are currently attracting considerable attention. These states represent neutral quasiparticles of the "electron plus hole" type with zero energy and non-Abelian quantum statistics, and are rather promising for use in quantum computations [2], [3], [5], [6].

In experiment, the occurrence MBSs is mainly related to the zero-bias differential conductance peak in the topological phase of a one-dimensional superconducting structure [7]–[10]. However, it turned out in recent years that a similar effect also arises in the trivial phase and is caused by the presence of Andreev

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bound states (ABSs) [11]–[14]. This raises the following question: what happens to bound states in transition from the topological to the trivial phase or vice versa? For instance, it is known that spins of both electron and hole components of quasiparticle states flip under such a transition [15], [16]. In a recent experiment [17], the occurrence of conductance peaks in a topological phase transition was studied. It turned out that as the superconducting gap closes in such a transition, the conductance peak is absent in the trivial phase and hence ABSs are also absent.

In this paper, we study three one-dimensional superconducting structures: 1) the one with classical p-wave superconductivity; 2) the main experimental model of a nanowire with s-wave superconductivity generated by the bulk superconductor due to the proximity effect in the presence of an external magnetic field and Rashba spin–orbit interaction; 3) the boundary of a two-dimensional topological insulator with an s-wave superconductivity order in an external magnetic field. To obtain precise analytic results, we consider not the SNS structure but its simplified model "superconductor–magnetic impurity–superconductor," with the impurity described by a delta-like potential. This leads to strongly overlapping wave functions; in particular, MBS-like bound states are not separated spatially, which precludes their use in applications. However, we note that, generally speaking, these states can be separated spatially via an external magnetic field [18], [19].

Using the Bogoliubov–de Gennes (BdG) equations, we study the behavior of stable states of the "electron"("hole") type for the first model and of the "electron plus hole" type for the other two models, which arise in the structures under consideration with the energies near the edges of the superconducting gap (see [20], [21]) as the system passes from the topological phase to the trivial one. As is known, the presence of a topological or trivial phase is determined by a relation between the system parameters, with the superconducting gap decreasing to zero at the instant of phase transition [2], [5]. It turned out that a major role is played in the phase transition by resonance (decaying) states, with the accompanying spin flip [15], [16] occurring not instantaneously, being related to the transition of bound quasiparticles to resonance ones and vice versa, with their energies changing to the opposite ones. Moreover, we explain the absence of ABSs in closing the gap in the trivial phase, as observed in experiment [17].

In what follows, ABS applies to any bound states, and MBS, to the zero-energy ABSs satisfying conjugation conditions (see (2) or (22) below); the standard spatially separated MBSs cannot arise in the framework of this simple model because of the overlap of wave functions.

2. Case of a *p*-wave superconducting order

The BdG Hamiltonian in the considered case has the form

$$H = \begin{pmatrix} -\partial_x^2 - \mu & -\Delta\partial_x \\ \Delta\partial_x & \partial_x^2 + \mu \end{pmatrix}, \tag{1}$$

where $\Delta \neq 0$ is a real parameter of the superconducting order and μ is the chemical potential. Hamiltonian (1) acts on functions of the form $\Psi(x) = (\psi_{\mathrm{e}}(x), \psi_{\mathrm{h}}(x))^{\mathrm{T}}$, where the superscript T denotes transposition; $\psi_{\mathrm{e}}(x)$ and $\psi_{\mathrm{h}}(x)$ are the electron and hole components. A zero-energy ABS is by definition an MBS if the conjugation condition

$$\psi_{\mathrm{e}}^*(x) = \psi_{\mathrm{h}}(x) \tag{2}$$

is satisfied [22].

Letting F denote the Fourier transformation, we write Hamiltonian (1) in momentum representation as

$$\widetilde{H}(p) - E = \begin{pmatrix} p^2 - \mu - E & -ip\Delta \\ ip\Delta & -p^2 + \mu - E \end{pmatrix},$$

where $\widetilde{H}(p) = FHF^{-1}$ and E is the quasiparticle energy. The dispersion law $\det(\widetilde{H}(p) - E) = 0$ has the form

$$E^2 = \left(p^2 - \mu + \frac{\Delta^2}{2}\right)^2 + \mu\Delta^2 - \frac{\Delta^4}{4}. \tag{3}$$

For $\mu < \Delta^2/2$, the spectrum of H is determined by the inequality $|E| \geq |\mu|$. We assume in what follows that

$$|\mu| \ll |\Delta|, \tag{4}$$

and hence the superconducting gap, equal to $(-|\mu|, |\mu|)$, is small. The Green's function of the Hamiltonian H has the form [21], [23]

$$G(x - x', E) = \begin{pmatrix} -g_+^{(1)} e^{ip_+|x-x'|} - g_-^{(2)} e^{ip_-|x-x'|} & \dfrac{\Delta}{4a}(e^{ip_+|x-x'|} - e^{ip_-|x-x'|}) \operatorname{sgn}(x - x') \\ -\dfrac{\Delta}{4a}(e^{ip_+|x-x'|} - e^{ip_-|x-x'|}) \operatorname{sgn}(x - x') & g_-^{(1)} e^{ip_+|x-x'|} + g_+^{(2)} e^{ip_-|x-x'|} \end{pmatrix}, \tag{5}$$

where

$$\begin{aligned} a &= \sqrt{E^2 + \frac{\Delta^4}{4} - \mu\Delta^2}, \qquad & p_\pm &= \sqrt{\mu \pm a - \frac{\Delta^2}{2}}, \\ g_\pm^{(1)} &= \frac{a - \Delta^2/2 \pm E}{4ip_+ a}, \qquad & g_\pm^{(2)} &= \frac{a + \Delta^2/2 \pm E}{4ip_- a}. \end{aligned} \tag{6}$$

We consider a perturbed Hamiltonian $H + V$, where the potential

$$V = Z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \delta(x) \tag{7}$$

describes the impurity; here, Z is a real parameter and $\delta(x)$ is the Dirac delta function.

We consider energies E of bound or resonance states (with a finite lifetime) such that

$$|E| < |\mu|. \tag{8}$$

Using (4), (6), and (8), we find

$$a = \frac{\Delta^2}{2} - \mu + \frac{E^2 - \mu^2}{\Delta^2}, \tag{9}$$

which by virtue of (6) yields

$$p_+ = \frac{i\sqrt{\mu^2 - E^2}}{|\Delta|}, \qquad p_- = i|\Delta|. \tag{10}$$

Consequently (see (5) and (6)), the points $E = \pm\mu$ are branching points of the Green's function $G(x-x', E)$. By (8), bound states are in correspondence with the positive square root in (10), and therefore their wave functions decrease exponentially. Resonance states lie on the second sheet of the Green's function; the minus sign appears in front of the square root in (10), and the wave functions increase exponentially. The lifetime of a state is inversely proportional to $|p_+|$ [24], [25] (see the end of this section for more details). We study both bound and resonance states using the Dyson equation

$$\Psi = -(H - E)^{-1} V \Psi. \tag{11}$$

We first assume that the system is in the topological phase $\mu > 0$ (see [2], [5]). Using (3)–(10), we write (11) in the form

$$\begin{aligned} \psi_{\rm e}(x) &= \frac{Z}{2\Delta}\biggl(\biggl(\sqrt{\frac{\mu-E}{\mu+E}}e^{ip_+|x|} - e^{ip_-|x|}\biggr)\operatorname{sgn}(\Delta)\psi_{\rm e}(0) + (e^{ip_+|x|} - e^{ip_-|x|})\operatorname{sgn}(x)\psi_{\rm h}(0)\biggr), \\ \psi_{\rm h}(x) &= \frac{Z}{2\Delta}\biggl((e^{ip_+|x|} - e^{ip_-|x|})\operatorname{sgn}(x)\psi_{\rm e}(0) + \biggl(\sqrt{\frac{\mu+E}{\mu-E}}e^{ip_+|x|} - e^{ip_-|x|}\biggr)\biggr)\operatorname{sgn}(\Delta)\psi_{\rm h}(0). \end{aligned} \tag{12}$$

We are interested in what follows only in stable ABSs arising for small Z. Setting $x = 0$ in (12), we see that system (12) has a nonzero solution if

$$\frac{Z}{2|\Delta|}\biggl(\sqrt{\frac{\mu-E}{\mu+E}} - 1\biggr) = 1, \qquad \psi_{\rm h}(0) = 0 \tag{13}$$

or

$$\frac{Z}{2|\Delta|}\biggl(\sqrt{\frac{\mu+E}{\mu-E}} - 1\biggr) = 1, \qquad \psi_{\rm e}(0) = 0. \tag{14}$$

We rewrite the first inequality in (13) in the form

$$2|\Delta|\sqrt{\mu+E} = Z(\sqrt{\mu-E} - \sqrt{\mu+E}).$$

Consequently, for small $Z > 0$, there exists the energy level (here and hereafter, we omit insignificant small terms)

$$E = -\mu\biggl(1 - \frac{Z^2}{2\Delta^2}\biggr), \tag{15}$$

which is localized near the lower edge of the gap. It follows from (10) and (15) that

$$p_+ = \frac{i|\mu||Z|}{\Delta^2} \tag{16}$$

(the value of p_- is the same in all cases). Using (12) and (13), we find the wave function for the lower level $\Psi(x) = (1,0)^{\rm T}e^{ip_+|x|}$, which is an electron-like weakly localized quasiparticle.

Equations (14) describe ABSs near the upper edge. We similarly find

$$E = \mu\biggl(1 - \frac{Z^2}{2\Delta^2}\biggr)$$

for small $Z > 0$, with the wave function $\Psi(x) = (0,1)^{\rm T}e^{ip_+|x|}$ describing a weakly localized hole-like quasiparticle.

For the trivial phase $\mu < 0$, we similarly obtain an equality for the upper level

$$E = |\mu|\biggl(1 - \frac{Z^2}{2\Delta^2}\biggr) \tag{17}$$

under the condition $Z < 0$. Equality (16) remains true and the wave function has the form $\Psi(x) = (1,0)^{\rm T}e^{ip_+|x|}$. The lower level is described by equality (17) with E replaced with $-E$ and $Z < 0$. Then $\Psi(x) = (0,1)^{\rm T}e^{ip_+|x|}$.

As $\mu > 0$ decreases to zero, two ABSs corresponding to two edge points of the energy gap form two states with a wave function independent of x, of the form $(1, \pm 1)^{\mathrm{T}}$ in the limit.

We note that in contrast to [21], where the quantity μ characterizing the phase and the energy gap was assumed to be constant, we here assume Z to be constant, whereas μ changes from positive to negative values for the phase transition to be realized. In the simple case of p-wave superconductivity, in contrast to Secs. 3 and 4, this does not lead to significant changes in either assumptions or the results in comparison with those in [20].

For definiteness, we consider the first equality in (13), describing the lower edge of the gap in the topological phase. It shows that for small μ, the ABS energy $\varepsilon = \mu + E$ measured from the lower gap edge is also small. We write this equality in the approximate form

$$\sqrt{\varepsilon} = \frac{\sqrt{\mu} Z}{\sqrt{2}|\Delta|}. \tag{18}$$

By virtue of (10), this implies

$$p_+ = \frac{i\sqrt{\varepsilon}\sqrt{2\mu}}{|\Delta|},$$

and the first equality in (12) can be approximately written in the form

$$\psi_{\mathrm{e}}(x) = \frac{Z\sqrt{2\mu}}{2\Delta\sqrt{\varepsilon}} e^{-\sqrt{\varepsilon}(\sqrt{2\mu}/|\Delta|)|x|}, \tag{19}$$

where $\sqrt{\varepsilon}$ is the particle momentum (relative to the gap edge). Up to some factors, the function $\psi_{\mathrm{e}}(x)$ is the Green's function of the Hamiltonian $-\partial_x^2$,

$$-\frac{1}{2ip} e^{ip|x-x'|}$$

at $x' = 0$. Passing to the second sheet of the Riemann surface of $\sqrt{\varepsilon}$ (which coincides with the Riemann surface of the Green's function) with a cut along $(0, \infty)$, i.e., adding 2π to the argument of the function $\sqrt{\varepsilon}$, we have the square root sign changing from $+$ to $-$. By (19), this leads to an exponential increase in the wave function, i.e., to a transformation of localized state to resonance ones; in accordance with (18), the sign of Z must be reversed for the level to exist.

Thus, in the topological phase, the first equation in (12) generates an electron-like ABS for $Z > 0$ and a resonance electron-like state for $Z < 0$ with the energies near the lower edge of the gap. Analogously, the second equation in (12) generates a hole-like ABS for $Z > 0$ and a resonance hole-like state for $Z < 0$, with the energies near the upper edge of the gap. In the trivial phase, electrons and holes exchange their positions and the signs of Z then reverse.

For $Z > 0$, in the transition from the topological phase to the trivial one, an electron on the lower gap edge and a hole on the upper edge transform into resonance states, such that the electron occurs on the upper edge and the hole on the lower one. The same happens for $Z < 0$ if we exchange the positions of bound and resonance states (see Fig. 1).

3. Superconducting s-wave nanowire

We consider the BdG Hamiltonian for a superconducting nanowire [2], [22], [26], [27] of the form

$$H_s = \begin{pmatrix} -\sigma_0\partial_x^2 + M\sigma_z - i\alpha\sigma_y\partial_x & i\sigma_y\Delta \\ -i\sigma_y\Delta & \sigma_0\partial_x^2 - M\sigma_z - i\alpha\sigma_y\partial_x \end{pmatrix}, \tag{20}$$

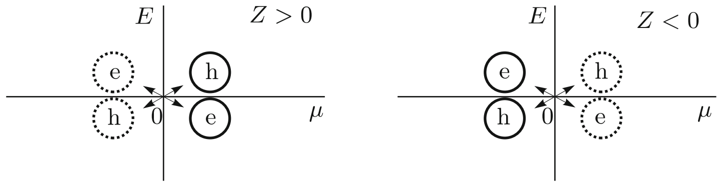

Fig. 1. Behavior of quasiparticles in the topological phase transition for p-wave superconductivity; e denotes an electron and h a hole, a solid border corresponds to a bound state and a dotted one to a resonance state.

where σ_0 is the 2×2 identity matrix, $\sigma_{x,y,z}$ are the Pauli matrices, $\Delta = \text{const} \neq 0$ is the superconducting order parameter, M describes the transverse Zeeman field, and α is the strength of the Rashba spin–orbit coupling. The Hamiltonian H_s describes a structure with s-wave superconductivity induced due to the proximity effect by the "parent" superconductor. The Hamiltonian acts on Nambu spinors of the form

$$\Psi(x) = (\psi_{\mathrm{e}\uparrow}(x), \psi_{\mathrm{e}\downarrow}(x), \psi_{\mathrm{h}\uparrow}(x), \psi_{\mathrm{h}\downarrow}(x))^{\mathrm{T}}, \tag{21}$$

where the arrow $\uparrow$ ($\downarrow$) denotes spin up (down), and the two first and the two last components respectively describe electrons and holes. By the MBS, we here understand a zero-energy ABS described by a wave function of form (21) and satisfying the conjugation conditions [1], [22], [28]

$$\psi_{\mathrm{e}\uparrow}(x)^* = \psi_{\mathrm{h}\downarrow}(x), \qquad \psi_{\mathrm{e}\downarrow}(x)^* = \psi_{\mathrm{h}\uparrow}(x). \tag{22}$$

We consider particles with small momenta p, and therefore we neglect quantities p^γ, $\gamma > 2$, in what follows.

In the momentum representation, we have

$$\widetilde{H}_s(p) = \begin{pmatrix} \sigma_0 p^2 + M\sigma_z + \alpha\sigma_y p - \sigma_0 E & i\sigma_y\Delta \\ -i\sigma_y\Delta & -\sigma_0 p^2 - M\sigma_z + \alpha\sigma_y p - \sigma_0 E \end{pmatrix}.$$

In the chosen approximation,

$$\det(\widetilde{H}_s(p) - E) = 2\alpha^2(M^2 - \Delta^2 - E^2)(p^2 - a^2),$$

where

$$a^2 = \frac{4\Delta^2 E^2 - (M^2 - \Delta^2 - E^2)^2}{2\alpha^2(M^2 - \Delta^2 - E^2)}. \tag{23}$$

The dispersion law $\det(\widetilde{H}_s(p) - E) = 0$ has the form [21]

$$E^2 = (\Delta \pm \sqrt{M^2 + \alpha^2 p^2}).$$

Consequently, the spectrum of H_s is described by the inequality $|E| \geqslant \big||M| - |\Delta|\big|$. The Green's function of H_s has the form [21]

$$G_s(x - x', E) = (g_{ij}(x - x', E))\big|_{i,j=1}^4,$$

where

$$
\begin{aligned}
g_{11}(x-x',E) = -g_{33}(x-x',-E) &= \frac{-(M+E)^2+\Delta^2+\alpha^2(M+E)}{2\alpha^2(M^2-\Delta^2-E^2)}\delta(x-x') - \\
&- \frac{(-(M+E)^2+\Delta^2+\alpha^2(M+E))a^2+(M-E)((M+E)^2-\Delta^2)}{4ia\alpha^2(M^2-\Delta^2-E^2)}e^{ia|x-x'|}, \\
g_{12}(x-x',E) = -g_{21}(x-x',E) &= g_{34}(x-x',E) = -g_{43}(x-x',E) = \\
&= \frac{1}{4\alpha}e^{ia|x-x'|}\operatorname{sgn}(x-x'), \\
g_{13}(x-x',E) = -g_{31}(x-x',E) &= g_{24}(x-x',E) = -g_{42}(x-x',E) = \\
&= \frac{E\Delta}{2\alpha(M^2-\Delta^2-E^2)}e^{ia|x-x'|}\operatorname{sgn}(x-x'), \\
g_{14}(x-x',E) = g_{41}(x-x',E) &= -g_{23}(x-x',-E) = -g_{32}(x-x',-E) = \\
&= \frac{\Delta}{2(M^2-\Delta^2-E^2)}\delta(x-x') + \frac{\Delta(\alpha^2a^2+(M+E)^2-\Delta^2)}{4ia\alpha^2(M^2-\Delta^2-E^2)}e^{ia|x-x'|}, \\
g_{22}(x-x',E) = -g_{44}(x-x',-E) &= \frac{-(M-E)^2+\Delta^2-\alpha^2(M-E)}{2\alpha^2(M^2-\Delta^2-E^2)}\delta(x-x') + \\
&+ \frac{((M-E)^2-\Delta^2+\alpha^2(M-E))a^2+(M+E)((M-E)^2-\Delta^2)}{4ia\alpha^2(M^2-\Delta^2-E^2)}e^{ia|x-x'|}.
\end{aligned}
\tag{24}
$$

We define the scalar product

$$(\psi,\varphi) = \int_{-\infty}^{\infty}\psi(x)\varphi^*(x)\,dx.$$

Let φ_0 be an even nonnegative continuous function that is nonvanishing only in a small neighborhood of the point $x=0$ and is such that

$$\int_{\mathbb{R}}\varphi_0(x)\,dx = 1.$$

In what follows, we consider the perturbed Hamiltonian H_s+V, where V is a separable potential (see [29], [30]) defined by the formula

$$(V\Psi)(x) = (V_m\Psi)(x) = m((\psi_{\mathrm{e}\uparrow},\varphi_0), -(\psi_{\mathrm{e}\downarrow},\varphi_0), -(\psi_{\mathrm{h}\uparrow},\varphi_0), (\psi_{\mathrm{h}\downarrow},\varphi_0))^{\mathrm{T}}\varphi_0(x) \tag{25}$$

or

$$(V\Psi)(x) = (V_Z\Psi)(x) = Z((\psi_{\mathrm{e}\uparrow},\varphi_0), (\psi_{\mathrm{e}\downarrow},\varphi_0), -(\psi_{\mathrm{h}\uparrow},\varphi_0), -(\psi_{\mathrm{h}\downarrow},\varphi_0))^{T}\varphi_0(x). \tag{26}$$

In (25), the potential V describes a local perturbation of the Zeeman field, and in (26), the impurity.

For functions that are slowly varying near zero, including the wave functions with small momenta considered below, a separable potential acts similarly to a delta function (the delta function itself cannot be used here because the term involving δ^2 appears in view of the structure of the Green's function).

We study eigenvalues and eigenfunctions of the Hamiltonian H_s+V, as in Sec. 2, using the Dyson equation

$$\Psi = -(H_s-E)^{-1}V\Psi. \tag{27}$$

We assume the conditions

$$M,\Delta,\alpha > 0, \qquad |M-\Delta| \ll M(\Delta), \alpha^2 \tag{28}$$

to hold and also assume the conditions for levels

$$|E| < (1+\sigma)|M-\Delta|, \qquad \sigma > 0 \tag{29}$$

(for the model considered in this section, energies of bound states can be outside the superconducting gap). From (23), (28), and (29), we then find

$$a^2 = \frac{\Delta(E^2-(M-\Delta)^2)}{\alpha^2(M-\Delta)} = O(M-\Delta). \tag{30}$$

Next, we have

$$\begin{aligned} &(M\pm E)^2-\Delta^2 = 2\Delta(M-\Delta\pm E)+O(M-\Delta)^2,\\ &M^2-\Delta^2-E^2 = 2\Delta(M-\Delta)+O(M-\Delta)^2. \end{aligned} \tag{31}$$

We first consider the case of the topological phase $M-\Delta>0$ (see [2], [5]). We assume that E is inside the energy gap, i.e., $|E/(M-\Delta)|<1$. Using (30) and (31), we reduce equalities (24) to the form

$$\begin{aligned} g_{11}(x-x',E) &= -g_{33}(x-x',-E) = \frac{1}{4(M-\Delta)}\delta(x-x')+\\ &\qquad + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{8\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}e^{ia|x-x'|},\\ g_{12}(x-x',E) &= -g_{21}(x-x',E) = g_{34}(x-x',E) = -g_{43}(x-x',E) =\\ &= \frac{1}{4\alpha}e^{ia|x-x'|}\operatorname{sgn}(x-x'),\\ g_{13}(x-x',E) &= -g_{31}(x-x',E) = g_{24}(x-x',E) = -g_{42}(x-x',E) =\\ &= \frac{E}{4\alpha(M-\Delta)}e^{ia|x-x'|}\operatorname{sgn}(x-x'),\\ g_{14}(x-x',E) &= g_{41}(x-x',E) = -g_{23}(x-x',-E) = -g_{32}(x-x',-E) =\\ &= -\frac{1}{4(M-\Delta)}\delta(x-x') - \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{8\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}e^{ia|x-x'|},\\ g_{22}(x-x',E) &= -g_{44}(x-x',-E) = -\frac{1}{4(M-\Delta)}\delta(x-x')-\\ &\qquad - \frac{\sqrt{\Delta}(1-E/(M-\Delta))^2}{8\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}e^{ia|x-x'|}. \end{aligned} \tag{32}$$

We introduce the notation $x_{\mathrm{e}\uparrow(\downarrow)} = (\psi_{\mathrm{e}\uparrow(\downarrow)},\varphi_0)$ and $x_{\mathrm{h}\uparrow(\downarrow)} = (\psi_{\mathrm{h}\uparrow(\downarrow)},\varphi_0)$. Choosing the potential in (25) and using (32), we write Dyson equation (27) in the form

$$\begin{aligned} \psi_{\mathrm{e}\uparrow} = \frac{m}{4}\biggl(&-\frac{x_{\mathrm{e}\uparrow}}{M-\Delta}\varphi_0(x) - \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2 x_{\mathrm{e}\uparrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}+\\ &+\frac{\operatorname{sgn}(x)e^{ia|x|}x_{\mathrm{e}\downarrow}}{\alpha}+\frac{E\operatorname{sgn}(x)e^{ia|x|}x_{\mathrm{h}\uparrow}}{\alpha(M-\Delta)}+\\ &+\frac{x_{\mathrm{h}\downarrow}}{M-\Delta}\varphi_0(x)+\frac{\sqrt{\Delta}(1+E/(M-\Delta))^2 x_{\mathrm{h}\downarrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\biggr),\\ \psi_{\mathrm{e}\downarrow} = \frac{m}{4}\biggl(&\frac{\operatorname{sgn}(x)e^{ia|x|}x_{\mathrm{e}\uparrow}}{\alpha}-\frac{x_{\mathrm{e}\downarrow}}{M-\Delta}\varphi_0(x)-\\ &-\frac{\sqrt{\Delta}(1-E/(M-\Delta))^2 x_{\mathrm{e}\downarrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}+\frac{x_{\mathrm{h}\uparrow}}{M-\Delta}\varphi_0(x)+\\ &+\frac{\sqrt{\Delta}(1-E/(M-\Delta))^2 x_{\mathrm{h}\uparrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}-\frac{E\operatorname{sgn}(x)e^{ia|x|}x_{\mathrm{h}\downarrow}}{\alpha(M-\Delta)}\biggr), \end{aligned}$$

$$
\begin{aligned}
\psi_{\mathrm{h}\uparrow} = \frac{m}{4}\biggl(&\frac{E\,\mathrm{sgn}(x)e^{ia|x|}x_{\mathrm{e}\uparrow}}{\alpha(M-\Delta)} + \frac{x_{\mathrm{e}\downarrow}}{M-\Delta}\varphi_0(x) + \\
&+ \frac{\sqrt{\Delta}(1-E/(M-\Delta))^2 x_{\mathrm{e}\downarrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}} - \frac{x_{\mathrm{h}\uparrow}}{M-\Delta}\varphi_0(x) - \\
&- \frac{\sqrt{\Delta}(1-E/(M-\Delta))^2 x_{\mathrm{h}\uparrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}} - \frac{\mathrm{sgn}(x)e^{ia|x|}x_{\mathrm{h}\downarrow}}{\alpha}\biggr), \\
\psi_{\mathrm{h}\downarrow} = \frac{m}{4}\biggl(&\frac{x_{\mathrm{e}\uparrow}}{M-\Delta}\varphi_0(x) + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2 x_{\mathrm{e}\uparrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}} + \\
&+ \frac{E\,\mathrm{sgn}(x)e^{ia|x|}x_{\mathrm{e}\downarrow}}{\alpha(M-\Delta)} + \frac{\mathrm{sgn}(x)e^{ia|x|}x_{\mathrm{h}\uparrow}}{\alpha} - \\
&- \frac{x_{\mathrm{h}\downarrow}}{M-\Delta}\varphi_0(x) - \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2 x_{\mathrm{h}\downarrow}e^{ia|x|}}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\biggr).
\end{aligned}
\tag{33}
$$

Multiplying Eqs. (33) by $\varphi_0(x)$ and setting $C = (\varphi_0, \varphi_0)$, we obtain two independent linear systems. The first system is

$$
\begin{pmatrix}
1 + \frac{m}{4}\left(\frac{C}{M-\Delta} + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\right) & -\frac{m}{4}\left(\frac{C}{M-\Delta} + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\right) \\
-\frac{m}{4}\left(\frac{C}{M-\Delta} + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\right) & 1 + \frac{m}{4}\left(\frac{C}{M-\Delta} + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\right)
\end{pmatrix} \times
$$

$$
\times (x_{\mathrm{e}\uparrow}, x_{\mathrm{h}\downarrow})^{\mathrm{T}} = 0, \tag{34}
$$

and the second system is obtained from (34) by replacing $E \to -E$, $(x_{\mathrm{e}\uparrow}, x_{\mathrm{h}\downarrow})^{\mathrm{T}} \to (x_{\mathrm{e}\downarrow}, x_{\mathrm{h}\uparrow})^{\mathrm{T}}$. We write the condition for the existence of a nonzero solution of system (34):

$$
1 + \frac{m}{2}\left(\frac{C}{M-\Delta} + \frac{\sqrt{\Delta}(1+E/(M-\Delta))^2}{2\alpha\sqrt{M-\Delta}\sqrt{1-(E/(M-\Delta))^2}}\right) = 0,
$$

which is equivalent to

$$
4\alpha(M-\Delta)\sqrt{1-\frac{E}{M-\Delta}} + 2\alpha m C\sqrt{1-\frac{E}{M-\Delta}} + m\sqrt{\Delta}\sqrt{M-\Delta}\left(1+\frac{E}{M-\Delta}\right)^{3/2} = 0. \tag{35}
$$

Let $m = \mathrm{const}$ and $M - \Delta \approx 0$; then (35) can be written in the form

$$
2\alpha C\sqrt{1-\frac{E}{M-\Delta}} = -\sqrt{\Delta(M-\Delta)}\left(1+\frac{E}{(M-\Delta)}\right)^{3/2}. \tag{36}
$$

Consequently, for the energy level to exist, the square root in the left-hand side of (36) must be negative. It follows from (36) that E is near the upper gap edge $M - \Delta$. By virtue of (36), we have

$$
4\alpha^2 C^2\left(1-\frac{E}{M-\Delta}\right) = \Delta(M-\Delta)\left(1+\frac{E}{M-\Delta}\right)^3. \tag{37}
$$

We set $x = 1 - E/(M-\Delta)$ and consider (37) as a fixed-point equation [31]

$$
x = f(x),
$$

where $f(x) = (\Delta/(4\alpha^2 C^2))(M-\Delta)(2-x)^3$. It is easy to see that the map $f(x)$ is a contraction in a neighborhood of zero [31]. The coefficient before $(2-x)^3$ is arbitrarily small, and we can therefore restrict ourself to the first approximation. As the zeroth approximation, it is natural to choose $x_0 = 0$, then the first approximation has the form $x_1 = 2\Delta(M-\Delta)/(\alpha^2 C^2)$. Thus, for a negative square root, equality (37) takes the form

$$\sqrt{1-\frac{E}{M-\Delta}} \approx -\frac{\sqrt{2\Delta(M-\Delta)}}{\alpha C}. \tag{38}$$

We note that formula (38) is significantly different from an analogous formula in [21], obtained for $M-\Delta = \text{const}$ and $m \to 0$.

With (38), Eq. (34) takes the form

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_{\mathrm{e}\uparrow} \\ x_{\mathrm{h}\downarrow} \end{pmatrix} = 0,$$

whence $x_{\mathrm{e}\uparrow} = -x_{\mathrm{h}\downarrow}$. We set $x_{\mathrm{e}\uparrow} = -x_{\mathrm{h}\downarrow} = 1$. By (30) and (38) (taking the sign of the square root in the left-hand side of (38) into account), we have $a = -i\sqrt{\varepsilon\Delta}/\alpha$, where $\sqrt{\varepsilon\Delta} > 0$, $\varepsilon = M - \Delta - E$ (up to a sign, ε is the energy measured from the upper edge of the energy gap). From (33), omitting terms with coefficients of the order of unity before exponentials and also neglecting the term $-m/(2(M-\Delta))\varphi_0(x)$, whose $L^2(-\infty,\infty)$ norm is finite, in contrast to that of the remaining term, we obtain

$$\psi_{\mathrm{e}\uparrow}(x) = -\psi_{\mathrm{h}\downarrow}(x) = -\frac{m\sqrt{\Delta}}{\alpha\sqrt{2\varepsilon}} e^{(\sqrt{2\varepsilon\Delta}/\alpha)|x|}. \tag{39}$$

Up to coefficients, expression (39) is the Green's function of the Hamiltonian $-\partial_x^2$ with the energy on the second sheet of the Riemann surface (see Sec. 2). Thus, the wave function of the considered state has the form $\Psi(x) = (1,0,0,-1)^{\mathrm{T}} e^{(\sqrt{2\varepsilon\Delta}/\alpha)|x|}$, and this is a resonance state.

For the energy near the lower gap edge $-(M-\Delta)$, we have Eq. (38) and the wave function $\Psi(x) = (0,1,-1,0)^{\mathrm{T}} e^{(\sqrt{2\varepsilon\Delta}/\alpha)|x|}$ with E replaced by $-E$.

In the limit $M-\Delta \to 0$, we obtain two states independent of x of the form $\Psi_1(x) = (1,0,0,-1)^{\mathrm{T}}$ and $\Psi_2(x) = (0,1,-1,0)^{\mathrm{T}}$.

Potential (26) generates no states inside the energy gap because the system determinant in (34) is equal to 1 when m is replaced with the corresponding $\pm Z$.

For the trivial phase, we have $M-\Delta < 0$ [2], [5]. In accordance with (30), we must then assume that $|E| > |M-\Delta|$, otherwise the wave functions are unrelated to either bound or resonance states.

In the trivial phase, the levels close to the lower gap edge are described by the equality

$$E = -|M-\Delta|\left(1 + \frac{2\Delta|M-\Delta|}{\alpha^2 C^2}\right), \tag{40}$$

and the wave function is localized and has the form $\Psi(x) = (1,0,0,-1)^{\mathrm{T}} e^{-(\sqrt{2\Delta}/\alpha)\sqrt{\varepsilon}|x|}$, where $\varepsilon = -E - |M-\Delta|$. For the upper edge, after replacing E with $-E$, the level is described by formula (40), $\Psi(x) = (0,1,-1,0)^{\mathrm{T}} e^{-(\sqrt{2\Delta}/\alpha)\sqrt{\varepsilon}|x|}$.

Thus, in closing the gap in the topological phase, the energy $E \approx M-\Delta$ of a resonance quasiparticle described by the wave function $(1,0,0,-1)^{\mathrm{T}} e^{(\sqrt{2\varepsilon\Delta}/\alpha)|x|}$, being localized inside the gap, vanishes (see Fig. 2), while the quasiparticle lifetime increases to infinity. Next, in the trivial phase, the energy decreases to below zero, going outside the gap to the continuum spectrum near the lower edge ($E \approx -(\Delta - M)$), with enhanced localization of the quasiparticle near $x = 0$. Similarly, the energy of a resonance quasiparticle with the wave

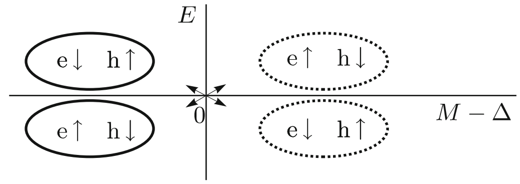

Fig. 2. Behavior of "electron plus hole" quasiparticles for the topological phase transition for s-wave superconductivity; the ↑ and ↓ arrows show the spin direction, e denotes an electron, h denotes a hole, a solid border corresponds to a bound state, and a dotted border to a resonance state.

function $(0,1,-1,0)^{\mathrm{T}} e^{(\sqrt{2\varepsilon\Delta}/\alpha)|x|}$ goes up along the E axis, and the quasiparticle becomes localized. In both cases, the electron and hole spins preserve their spin direction. There is no immediate spin flip; the change in the spin direction is a consequence of the process in which the quasiparticles exchange their positions.

For $M-\Delta \approx 0$, we can make this model closer to a more realistic s-wave nanowire model describing the "normal metal–superconductor–normal metal" structure, where the length of the superconducting section is sufficiently large. For this, we should extend the domain of the local magnetic field and, varying the parameter m, go over to another phase in this domain (see [18], [19]). Then the two overlapping states with the energies near the gap edges, being Majorana-like, must move to two respective boundary points of the domain with the local field, because the topological phase changes at these points.

For the trivial phase with potential (25), quasiparticle energies are outside the gap and lie in the continuum spectrum; such localized particles are unstable and readily transform into resonance states [32], whereas there are no stable localized states inside the gap. Thus, for the topological phase transition from the trivial phase to the topological one, the conductance peak must be absent until the gap closes, which is confirmed by experiment [17]. On the other hand, in the topological phase with a very small energy gap, the lifetime of resonance quasiparticles with the energies within the gap is almost infinite, and these particles are therefore capable of generating the conductance peak, which is indeed observed in experiment.

4. The case of a superconducting boundary of a topological insulator

We consider the BdG Hamiltonian for an s-wave superconducting boundary of a two-dimensional topological insulator [5], [22], [33]–[36]

$$H_{\mathrm{TI}} = \begin{pmatrix} -i\sigma_x\partial_x + M\sigma_z & i\sigma_y\Delta \\ -i\sigma_y\Delta & -i\sigma_x\partial_x - M\sigma_z \end{pmatrix}, \tag{41}$$

where $\Delta = \text{const} \neq 0$ is a real pairing potential and M is the parameter of the transverse Zeeman field. Hamiltonian (41), as in Sec. 3, acts on spinors of form (21). The dispersion law is

$$E^2 = (M \pm \Delta)^2 + p^2, \tag{42}$$

and the spectrum of H_{TI} is therefore determined by the inequality $|E| \geqslant \big||M| - |\Delta|\big|$.

As in the foregoing, in order to find energy levels E and the corresponding wave functions, we use the Dyson equation

$$\Psi = -(H_{\mathrm{TI}} - E)^{-1} V \Psi, \tag{43}$$

where

$$V = V_m = m \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix} \delta(x) \tag{44}$$

or

$$V = V_Z = Z \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix} \delta(x), \tag{45}$$

with σ_0 being the unit 2×2 matrix. Potential (44) models variations in the local Zeeman field, and potential (45) models the impurity. The Green's function of H_{TI} has the form [20]

$$G(x-x', E) = \frac{1}{4} \begin{pmatrix} g_E^+(x-x') & g^+(x-x') & g^-(x-x') & g_E^-(x-x') \\ g^+(x-x') & -g_{-E}^+(x-x') & -g_{-E}^-(x-x') & g^-(x-x') \\ g^-(x-x') & -g_{-E}^-(x-x') & -g_{-E}^+(x-x') & g^+(x-x') \\ g_E^-(x-x') & g^-(x-x') & g^+(x-x') & g_E^+(x-x') \end{pmatrix}, \tag{46}$$

where

$$\begin{aligned} g_E^{\pm}(x-x') &= \sqrt{\frac{M+\Delta+E}{M+\Delta-E}} e^{ip_1|x-x'|} \pm \operatorname{sgn}(M-\Delta) \sqrt{\frac{M-\Delta+E}{M-\Delta-E}} e^{ip_2|x-x'|}, \\ g^{\pm}(x-x') &= i\big(e^{ip_1|x-x'|} \pm e^{ip_2|x-x'|}\big) \operatorname{sgn}(x-x'), \end{aligned}$$

and $p_{1,2}$ are found from law (42) such that the Green's function decrease at infinity.

We assume in what follows that $M, \Delta > 0$, $|M-\Delta| \ll M(\Delta)$ and $|E| < |M-\Delta|$. It then follows from (42) that

$$\begin{aligned} p_1 &= \pm\sqrt{E^2 - (M+\Delta)^2} \approx \pm 2i\Delta, \\ p_2 &= \pm\sqrt{E^2 - (M-\Delta)^2} \approx \pm i\sqrt{(M-\Delta)^2 - E^2}. \end{aligned} \tag{47}$$

We consider the Hamiltonian with potential (44) for the topological phase $\Delta - M > 0$ [2], [5]. We seek the ABS energies near the gap edges, assuming that $|E| < \Delta - M$. We set $\varepsilon = \Delta - M - E$. Using (46) and (47) and neglecting terms with coefficients of the order of unity and higher in the parameter ε, we write Green's function (46) in the form

$$G(x-x', E) = \frac{\sqrt{\Delta - M} e^{ip_2|x-x'|}}{2\sqrt{2\varepsilon}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{48}$$

By virtue of (44) and (48), Dyson equation (43) becomes

$$\psi_{\mathrm{e}\downarrow}(x) = -\psi_{\mathrm{h}\uparrow}(x) = \frac{m\sqrt{\Delta - M} e^{ip_2|x|}}{2\sqrt{2\varepsilon}} (\psi_{\mathrm{e}\downarrow}(0) - \psi_{\mathrm{h}\uparrow}(0)). \tag{49}$$

For small $m > 0$, we write the condition for the existence of a nonzero solution of system (49):

$$1 - \frac{m\sqrt{\Delta - M}}{\sqrt{2\varepsilon}} = 0. \tag{50}$$

It follows from (50) that

$$E = (\Delta - M)\left(1 - \frac{m^2}{2}\right) \approx \Delta - M. \tag{51}$$

By virtue of (47) and (49), the ABS wave function has the form

$$\Psi(x) = (0, 1, -1, 0)^{\mathrm{T}} e^{-\sqrt{2\varepsilon(\Delta - M)}|x|}.$$

Replacing E with $-E$, we use (51) to obtain a formula for the level $E \approx -(\Delta - M)$ and also an expression for the wave function of the corresponding ABS:

$$\Psi(x) = (1, 0, 0, -1)^{\mathrm{T}} e^{-\sqrt{2\varepsilon(\Delta - M)}|x|}$$

for $m < 0$ (the change of sign of m is determined by the type of potential (44)).

In the trivial phase, $M - \Delta > 0$ and the Green's function takes form

$$G(x - x', E) = \frac{\sqrt{M - \Delta}e^{ip_2|x-x'|}}{2\sqrt{2\varepsilon}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix},$$

where $\varepsilon = M - \Delta - E > 0$. As above, for $E \approx M - \Delta$, we obtain the level existence condition

$$1 + \frac{m\sqrt{M - \Delta}}{\sqrt{2\varepsilon}} = 0, \tag{52}$$

which implies that m is small and $m < 0$. We write the wave function

$$\Psi(x) = (1, 0, 0, -1)^{\mathrm{T}} e^{-\sqrt{2\varepsilon(M - \Delta)}|x|}.$$

For $E \approx -(M - \Delta)$, we have $m > 0$, in (52) and with E changed to $-E$ in ε the wave function takes form $\Psi(x) = (0, 1, -1, 0)^{\mathrm{T}} e^{-\sqrt{2\varepsilon(M-\Delta)}|x|}$.

In all the cases considered above, the Green's function for the boundary of a topological insulator involves the expression

$$\frac{\sqrt{|M - \Delta|}}{2\sqrt{2\varepsilon}} e^{-\sqrt{2\varepsilon|M-\Delta||x-x'|}}, \tag{53}$$

where ε is, up to sign, the energy near the gap edge. Similarly to the previous sections, expression (53) is (up to constant factors) the Green's function of the operator $-\partial_x^2$. In passing to the second sheet of the Riemann surface of the Green's function $G_{\mathrm{TI}}(x - x', E)$, the sign of $\sqrt{\varepsilon}$ changes, and hence, by virtue of (50) and (52) with the simultaneous change of sign of m, the quasiparticle undergoes a transition to a resonance state.

For potential (45), similarly to Sec. 3, the Dyson equation has no nonzero solutions.

Thus, for $m > 0$, under the transition from the topological to the trivial phase, an ABS with the energy near the upper gap edge transforms into an ABS with the energy near the lower edge such that the electron and hole spins are preserved, and the resonance quasiparticle with opposite spins and with the energy near the lower edge transforms into a resonance quasiparticle with the energy near the upper edge. For $m < 0$, the same takes place, but the resonance and localized quasiparticles exchange their positions (see Fig. 3).

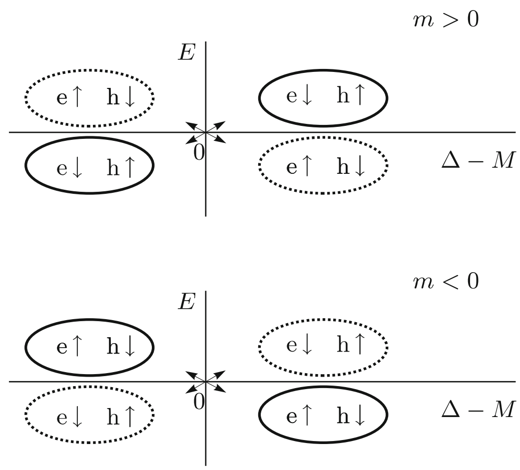

Fig. 3. Behavior of "electron plus hole" quasiparticles for the topological phase transition in the case of a topological insulator for different signs of the parameter m; the ↑ and ↓ arrows show the spin direction, e denotes an electron and h denotes a hole. A solid border corresponds to a bound state, and a dotted border, to a resonance state.

5. Conclusions

We have considered one-dimensional superconducting structures that are most popular in studies of Majorana states. Using the Green's functions of the BdG Hamiltonian and the Dyson equation, we analytically studied the energy levels and wave functions of stable states arising in such structures under a perturbation of the Hamiltonian with energies near the superconducting gap edges for the transition from the topological to the trivial phase. Resonance (decaying) states turned out to play a major role in the phase transition; the accompanying spin flip and sign reversal of the charge [15], [16] occur as the gap closes due to the transition of localized states to resonance ones and vice versa, with their energies changing to the opposite ones (see Figs. 1–3). Our results are consistent with the absence of the conductance peak for zero potential difference in the trivial topological phase in a recent experiment in [17].

Conflicts of interest. The authors declare no conflicts of interest.

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