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Anomalous superconducting proximity effect and coherent charge transport in semiconducting thin film with spin-orbit interaction

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Abstract – We present a microscopic theory of the superconducting proximity effect in a semiconducting thin film with a spin-orbit interaction (N_{SO}) in an external magnetic field. We demonstrate that an effective 1D Hamiltonian which describes induced superconductivity in N_{SO} in contact with a usual *s*-wave superconductor possesses not only a spin-singlet induced superconducting order parameter term, as commonly adopted, but also a spin triplet order parameter term. Using this new effective Hamiltonian we confirm previous results for a normal current across contacts of N_{SO} with a normal metal and for a Josephson current with the same N_{SO} with induced superconductivity, obtained previously in the framework of the phenomenological Hamiltonian without spin-triplet terms. However, a calculated current-phase relation across the transparent contact between N_{SO} with induced superconductivity in magnetic field and a usual *s*-wave superconductor differs significantly from previous results. We suggest the experiment which can confirm our theoretical predictions.

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How is it possible to describe the superconductivity induced in materials without attractive electron-electron interaction? The answer is well-known for the case of the contact between a normal metal and a usual s-wave spinsinglet superconductor (S) [1,2]. In this case the induced superconductivity in the metal without electron-electron attraction can be described by almost the same Hamiltonian as in the usual superconductor [1]. However, the type of the effective Hamiltonian which can describe the induced superconductivity in a semiconducting thin film with spin-orbit interaction (N_{SO}) is less evident. The hybrid structures based on usual s-wave superconductor and the semiconducting thin film $(S/N_{SO} \text{ contact})$ (fig. 1(a)) are very interesting from both the fundamental and the practical point of view due to the possibility to find in them zero-energy Majorana modes [3]. The microscopical self-consistent calculations of the proximity effect in such structures [4–7] were resricted to find just averaged pairing

amplitudes, *i.e.* Green function components, but not an effective Hamiltonian. Existing attempts of derivation of the effective Hamiltonian [3,8,9] describe the connection between the usual s-wave superconductor and the N_{SO} -film in terms of the tunnel Hamiltonian in the momentum space which does not permit to take into account the finite width of the N_{SO} -film, coherent reflections between boundaries as well as scattering between spin bands. Naturally, the important features of the effective Hamiltonian as triplet pairing component and momentum dependence of pairing component were missed.

In this letter, based on our tight-binding approach [10, 11] we demonstrate that the effective 1D Hamiltonian of S/N_{SO} structure in the basis $\Psi = (\Psi^{SO,\uparrow}, \Psi^{SO,\downarrow}, \bar{\Psi}^{SO,\uparrow}, \bar{\Psi}^{SO,\downarrow})$ should have the following form:

$$\widehat{H}_{eff} = \begin{pmatrix} \xi - h & \lambda k_y & \Delta_1(k_y) & \Delta_2(k_y) \\ \lambda k_y & \xi + h & -\Delta_2(k_y) & \Delta_3(k_y) \\ \Delta_1(k_y) & -\Delta_2(k_y) & -\xi + h & \lambda k_y \\ \Delta_2(k_y) & \Delta_3(k_y) & \lambda k_y & -\xi - h \end{pmatrix}, \quad (1)$$

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Fig. 1: (Colour online) Schematic illustration of the structure under consideration of the S/N_{SO} and N_{SO}/X junctions, where X is N, S or N_{SO} with induced superconductivity (a); tight-binding model of the proximity effect in the z-direction for S/N_{SO} junction (b).

instead of the widely used Hamiltonian [3,8,9,12] without triplet terms $\Delta_1(k_y) = \Delta_3(k_y) = 0$ and without momentum dependence of the induced singlet order parameter $\Delta_2(k_y) = \text{const. In eq. (1) } \xi \text{ is a single-particle excitation}$ energy, h is the Zeeman energy related to the magnetic field B applied in the z-direction (fig. 1(a)), $h = q_e^* \mu_B B/2$, g_e^* is the Landé factor, μ_B is the Bohr magneton, λ is a spin-orbit constant (we consider the Rashba model [13]) and k_u is a momentum parallel to the interface. Using this effective Hamiltonian (1) we demonstrate that it leads to well-known results for normal current for the contact with a normal metal $(N/S_{SO}$ junction) [14–16], where S_{SO} means a metal with spin-orbit interaction with induced superconductivity, and for the Josephson current for the symmetric junction with the same metal with induced superconductivity $(S_{SO}/c/S_{SO}$ Josephson junction) [17]. However, we demonstrate that the use of the Hamiltonian (1) leads to very unusual current-phase relations for the contact of this heterostructure (fig. 1(a)) with usual s-wave superconductor $(S/c/S_{SO}$ Josephson junction).

We consider the S/N_{SO} heterostructure which is depicted in fig. 1(a), (b). We suppose that S/N_{SO} boundary is sufficiently smooth, so the momentum parallel to the interface is conserved. The wave function in S material corresponding to the case of the bound states with $E < \Delta_0$ has the usual form [18]. We consider transport in the y-direction as depicted in fig. 1(a). In this case, an electron part of N_{SO} Hamiltonian has the following form [3,19]: $H_{SO} = \xi - h\tau_z + \lambda k_y \tau_x$, where $\tau_{x,z}$ are Pauli matrices, which corresponds to the left upper 2 × 2 submatrix of matrix (1). The lower right 2 × 2 submatrix of matrix (1) corresponds to the hole part of N_{SO} Hamiltonian. The wave functions of this electron-hole Hamiltonian without pairing terms have the form of the superposition of eight bispinors [20].

To solve the problem of the induced superconductivity in N_{SO} we should match wave functions on boundaries. In the tight-binding approximation it is suitable to use the boundary conditions for S/N_{SO} interface at $n_z = 0$ [10]. n_z means the number of atoms in the tight-binding scheme (fig. 1(b)), which corresponds to the coordinate z by the following relation $z = a \cdot n_z$, where a is the distance between atoms. For simplicity we put a = 1 in the remaining part of this letter. Open boundary of N_{SO} to vacuum corresponds to $n_z = N_z$. For spin-up components of the wave function these boundary conditions have the following form:

$$\begin{cases} t'\Psi_1^{S,\uparrow} = \gamma \Psi_1^{SO,\uparrow}, \\ t'\bar{\Psi}_1^{S,\uparrow} = \gamma \bar{\Psi}_1^{SO,\uparrow}, \\ t\Psi_0^{SO,\uparrow} = \gamma \Psi_0^{S,\uparrow}, \\ t\bar{\Psi}_0^{SO,\uparrow} = \gamma \bar{\Psi}_0^{S,\uparrow}, \end{cases}$$
(2)

where t, t', γ are tight-binding hopping amplitudes in N_{SO} , S and across boundary, respectively (fig. 1(b)). For spin-down components boundary conditions are similar to eq. (2), and for open boundary at $n_z = N_z$ one has the following boundary conditions: $\Psi_{N_z}^{SO,\uparrow} = \Psi_{N_z}^{SO,\downarrow} = \bar{\Psi}_{N_z}^{SO,\downarrow} = \bar{\Psi}_{N_z}^{SO,\downarrow} = 0$. In these boundary conditions, $\Psi_{n_z}^{X,\uparrow(\downarrow)}$ corresponds to the electron component of the wave function in X with spin up (down) on the atom with number n_z , $\bar{\Psi}_{n_z}^{X,\uparrow(\downarrow)}$ corresponds to the hole component of the wave function in X with spin up (down) on the atom with number n_z , where X is N_{SO} or S. The wave function matching method is similar to the one described in ref. [1], except that we additionally consider spin degrees of freedom.

Substitution of the wave functions to the boundary conditions eq. (2) leads to the transcendental equation, whose solution allows to obtain the induced excitation spectrum in N_{SO} . The obtained induced excitation spectra are rather similar to the previously obtained results with the phenomenological Hamiltonian [19,21]. For the case without magnetic field and for values of the magnetic field smaller than critical there are two gaps in the excitation spectrum: the first gap corresponds to the smaller value of k_y (Δ_2 in notation of ref. [19]) and the second gap corresponds to the larger value of k_y (Δ_1 in notation of ref. [19]). At critical value of the Zeeman field $h = h_c$ the first gap is closed, and then for values of the magnetic field larger than critical the first gap is reopened [12].

However, the Majorana states can arise at the end of the clean N_{SO} [17,22]. Therefore, the investigation of the transport in y-direction of N_{SO} (fig. 1(a)) is of great interest. The most common way to do it is to construct the effective 1D Hamiltonian using obtained wave functions. For this purpose one needs to construct the Green function for the lowest subband of N_{SO} [1] and then find the effective 1D Hamiltonian from the equation $-\hat{H}_{eff}(k_y)\hat{G}(k_y) = 1$. The components of the retarded Green function presented by 4×4 matrix are expressed through the components of the wave functions



Fig. 2: (a) The dependences of the induced triplet and singlet superconducting order parameters near the second gap on the wave vector for the value of the Zeeman field $h = 2 \Delta_0$ larger than the critical value, $\mu = 1215 \Delta_0$. (b) The dependences of the induced triplet and singlet superconducting order parameters near the second gap on the transparency of the interface D for the value of the Zeeman field $h = 2 \Delta_0$ larger than the critical value for $k_y = 0.845$, which corresponds to the second gap. The solid thick line corresponds to the triplet component Δ_3 , the dashed line to the triplet component Δ_1 and the solid thin line to the singlet component Δ_2 .

$$\Psi_{n_z}^{(\alpha)}(E_i(k_y), k_y) \ [1]:$$

$$G_{n_z, n_z}^{R, (\alpha\beta)}(k_y) = \sum_{i=1, \dots, 4} \frac{\langle \Psi_{n_z}^{(\alpha)}(E_i(k_y), k_y) \Psi_{n_z}^{(\beta)*}(E_i(k_y), k_y) \rangle}{E + i0 - E_i},$$
(3)

where $\alpha, \beta = 1, 2, 3, 4$, the sum is taken over all four branches of the induced spectrum, the brackets denote averaging over n_z $(1 \leq n_z \leq N_z)$. The obtained effective 1D Hamiltonian is presented by eq. (1) with nonzero triplet terms $\Delta_1(k_y)$ and $\Delta_3(k_y)$. We have checked the correctness of the obtained effective Hamiltonian with pairing terms by comparison of the obtained electron and hole parts of this Hamiltonian (the upper left 2×2 submatrix of matrix (1) and the lower right 2×2 submatrix of matrix (1) with initial submatrices. The calculated and initial electron and hole parts coincide, so we can conclude that our procedure is correct. The calculated triplet components $\Delta_1(k_y)$ and $\Delta_3(k_y)$ are odd functions of k_y , while the singlet component $\Delta_2(k_y)$ is an even function of k_y .

Our calculations demonstrate that even for the case B = 0 the induced triplet components are nonzero, have significant k_y dependences and satisfy the relation $\Delta_1(k_y) = -\Delta_3(k_y) = -\Delta_2(k_y)$ near the first gap and $\Delta_1(k_y) = -\Delta_3(k_y) = \Delta_2(k_y)$ near the second gap. The nonzero triplet components arise due to the presense of the spin-orbit interaction in the layer of N_{SO} with finite thickness where coherent reflections on the boundaries exist.

The applied magnetic field breaks the above-mentioned relations between induced singlet and triplet order parameter components. However, these components both exist for all values of magnetic field with strong dependence on the momentum k_y near gaps.

The dependences of the induced triplet and singlet superconducting order parameters near the second gap on the wave vector for the value of the Zeeman field $h = 2\Delta_0$ larger than the critical value are depicted in fig. 2(a), and the dependences of the induced triplet and singlet superconducting order parameters near the second gap on the transparency of the interface are depicted in fig. 2(b) for the same value of the magnetic field for $k_y = 0.845$ which corresponds to the second gap. From this figure one can see that for almost all values of transparency of the interface the magnitudes of the components of the induced order parameter are larger than the magnitude of the order parameter Δ_0 in S. However, it is possible to demonstrate that the measurable parameter, *i.e.* the gap in the induced spectrum, is always smaller than Δ_0 .

Using the effective 1D Hamiltonian (1) we have calculated the current-voltage characteristics (IVC) of the N/S_{SO} junction in the y-direction (fig. 1(a)) in the framework of the approach [10]. We demonstrate that at high Zeeman field $h > h_c$ zero-energy singularity in the IVC appears, which can be interpreted as zero-energy Majorana states. Thus, our results do not contradict to the previous results [14–16], where Majorana states and corresponding zero-energy singularities in the IVC of the N/S_{SO} junction were predicted.

However, the crucial experiment to determine the surface bound states is the Josephson tunneling experiment. With the aim to plan such experiment we have calculated Andreev bound states and the Josephson current in different short (the length of the junction is much smaller than the coherence length) superconducting junctions containing S_{SO} .

We have calculated Andreev bound states for the symmetric Josephson $S_{SO}/c/S_{SO}$ junction, which are presented in fig. 3(a). Thick solid and dashed lines in fig. 3(a) correspond to the transparency of the interface D = 0.145, the thin solid and dashed lines correspond to the transparency of the interface D = 1. It follows from fig. 3(a) that the 4π periodicity of the Josephson current-phase relation exists for any values of the transparency of the interface. Thus, our calculations confirm previous results for the Josephson current in symmetric superconducting $S_{SO}/c/S_{SO}$ junctions [17] which were obtained using a phenomenological Hamiltonian without triplet terms $\Delta_1(k_y) = \Delta_3(k_y) = 0$ and without momentum dependence of the induced singlet order parameter $\Delta_2(k_y) = \text{const in eq. (1)}.$



Fig. 3: (a) Andreev bound states for the $S_{SO}/c/S_{SO}$ junction; the thick solid and dashed lines correspond to the transparency of the interface D = 0.145, the thin solid and dashed lines to D = 1; (b) the current-phase relation for the $S/c/S_{SO}$ junction for the following values of parameters $t = t_S = -200\Delta_0$, $\lambda = 18\Delta_0$, $\mu = 398\Delta_0$, $h = 5\Delta_0$, $k_S = 2.5$, $\gamma = -200\Delta_0$, D = 0.135, $I_0 = 2e\Delta_{SO}/\hbar$; (c) the current-phase relation for the $S/c/S_{SO}$ junction for the same values of parameters as in (b) but $k_S = 0.25$, $\gamma = -180\Delta_0$, D = 0.83; (d) the current-phase relation for the $S/c/S_{SO}$ junction for the same values of parameters as in (b) but $k_S = 0.25$, $\gamma = -80\Delta_0$, D = 0.05.

However, an investigation of the current-phase relation of *asymmetric* short Josephson junctions, one bank of which is S_{SO} , and another bank is S, provides the possibility to distinguish between phenomenological and microscopically obtained Hamiltonians. In fig. 3(b)-(d) current-phase relations of asymmetric $S/c/S_{S0}$ Josephson junctions calculated from Hamiltonian (1) are presented for different values of $S/c/S_{S0}$ interface transparency. One can see that for relatively large values of S/S_{S0} interface transparency (D = 0.135 in fig. 3(b) and D = 0.83 infig. 3(c)) the calculated current-phase relations are rather unusual and significantly differ from well-known dependences. These dependences correspond to the order parameter symmetry breaking on the boundary in the case of asymmetric $S/c/S_{S0}$ Josephson junction. The same unusual current-phase dependences arise also in asymmetric contacts between usual s-wave superconductor and the superconductor with interband pairing [23]. The current-phase relation of a $S/c/S_{S0}$ Josephson junction with small S/S_{S0} interface transparency (fig. 3(d)) demonstrates usual sinusoidal dependence. Therefore, an investigation of current-phase relations of quite transparent asymmetric $S/c/S_{S0}$ Josephson junctions provides a possibility to verify our results.

We now discuss the design of an asymmetric $S/c/S_{S0}$ Josephson junction and a possible experimental setup for measuring the predicted effects. The Josephson junction we propose is based on a high-mobility AlGaSb/InAs/ AlGaSb heterostructure and niobium electrodes [24,25]. The hybrid nanostructure is defined by electron beam

lithography, selective reactive ion etching, and Nb sputter deposition. Only the top AlGaSb layer is etched in the central part of a semiconductor mesa of the hybrid nanostructure, while the InAs channel continues underneath a top niobium layer [24,25]. The etched semiconductor mesa (with the Nb layer on top) is laterally contacted to the superconducting niobium lead [26]. Highly transparent contacts can be formed in the junction by exploiting an Ar plasma cleaning of the contact area prior to the Nb sputter deposition [24–26]. The mean free path in the InAs quantum well $l_e > 3 \,\mu \text{m}$ [24,25], allowing for ballistic transport in nanostructures. The current-phase relation of the asymmetric Josephson junction can be determined by incorporating the junction into a superconducting loop coupled to a dc SQUID, allowing measurement of the junction phase difference [27, 28].

In summary, we present here a microscopic theory of the superconducting proximity effect in the contact of usual s-wave superconductor with a metal with spin-orbit interaction in an applied magnetic field. Our theory takes into account scattering between spin bands at the boundaries and finite size of the metal, which were missed in the previous investigation of the proximity effect in such structures [3,8,9]. We obtain the effective 1D Hamiltonian (1) which describes the induced superconductivity in such metal and demonstrates the presence of the spin-triplet order parameter components in it which contradicts previous investigations where only spin-singlet component were obtained [3,8,9]. Nevertheless, using the effective Hamiltonian (1) does not frustrate the main results obtained

previously for such materials: we confirm the existence of zero-energy bound state on the boundary of this material with a normal metal [14–16] and a 4π periodicity of the Josephson current in a symmetric junction [17]. At the same time, we show that the Josephson current-phase dependence of quite transparent contact of this material with conventional *s*-wave superconductors in magnetic fields is rather unusual. We suggest an experiment which can confirm the existence of triplet pairing terms in 1D effective Hamiltonian of a N_{SO} in contact with usual superconductor.

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