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Unconventional pairing in three-dimensional topological insulators with warped surface state

A. S. Vasenko[a1)], A. A. Golubov[b,c], V. M. Silkin[d,e], E. V. Chulkov[d,f]

[a]National Research University Higher School of Economics, 101000 Moscow, Russia

[b]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

[c]Moscow Institute of Physics and Technology, Dolgoprudny, 141700 Moscow, Russia

[d]Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU, 20080 San Sebastián, Basque Country, Spain

[e]IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

[f]Tomsk State University, 634050 Tomsk, Russia

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Three-dimensional topological insulators (3D TI) represent a new state of matter [1]. Their hallmark is the formation of conducting surface states with the Dirac dispersion relation, whereas the bulk states are gapped. Recently a lot of interest has been attracted to the physics of hybrid structures involving topological insulators and superconductors, where in presence of a magnetic field a Majorana fermion state can be realized [2]. When the 3D topological insulator is placed in the electrical contact with the s-wave superconductor (S), the superconducting pair correlations penetrate into the topological state due to the proximity effect. In accordance with the Pauli principle, it is customary to distinguish four classes of symmetry of the induced pair potential [3] (see Table 1).

Previously, the symmetry of the induced pair potential in S/TI junctions was studied on the basis of a simplified model, when the topological surface states were described with an isotropic Dirac cone. The Hamiltonian of surface states in this model reads $\hat{H}_0(\mathbf{k}) = -\mu + v(k_x\hat{\sigma}_y - k_y\hat{\sigma}_x)$. Here μ is a chemical potential, v is a Fermi velocity, $\mathbf{k} = (k_x,\ k_y)$ denotes in-plane quasiparticle momentum, and $\hat{\sigma}_j$ are the Pauli matrices ($j = x, y, z$). However, such isotropic forms of the Hamiltonian are only valid if the chemical potential lies near the Dirac point. In realistic topological insulators it usually lies well above this point, where the Dirac cone is strongly anisotropic and its constant energy contour has a snowflake shape [4]. This type of dispersion was described by adding higher order terms in the momentum to the Hamiltonian, $\hat{H}(\mathbf{k}) = \hat{H}_0(\mathbf{k}) + \hat{\sigma}_z\lambda k^3\cos(3\theta)$, where $\theta = \arctan(k_y/k_x)$ and λ is the hexagonal warping strength [4].

In this work we consider a superconductor/ferromagnetic insulator/topological insulator (S/FI/TI) junction along the z-direction. The structure is uniform in the x-y plane. The FI interlayer is thin enough, so that the superconducting correlations can penetrate the TI surface states due to the proximity effect. The ferromagneic insulator layer is located at $z = 0$, while topological insulator lies in $z < 0$ half-plane and the superconductor layer in $z > 0$ half-plane. The Hamiltonian for the TI surface states can be written as (we use "check" for 4×4 and "hat" for 2×2 matrices),

$$\check{H}_S(\mathbf{k}) = \begin{pmatrix} \hat{H}(\mathbf{k}) + \hat{\sigma}_z M & \hat{\Delta} \\ -\hat{\Delta} & -\hat{H}^*(-\mathbf{k}) - \hat{\sigma}_z M \end{pmatrix}. \quad (1)$$

Here $\hat{\Delta} = \mathrm{i}\hat{\sigma}_y\Delta$, where Δ is the superconducting pair potential, induced in the topological insulator surface due to the proximity effect, and M is the exchange field of the ferromagnetic insulator, which we consider to be perpendicular to the topological surface.

To obtain the energy dispersion relation of topological surface states we start with the following equation, $\left[E - \check{H}_S(\mathbf{k})\right]\check{G} = \check{1}$, where $\check{G}$ is the Green's function on the TI surface, $\check{1}$ is the unitary 4×4 matrix, and E is the quasiparticle energy counted from the chemical potential. By taking the inverse of this equation we can obtain the Green's function,

$$\check{G} = \begin{pmatrix} \hat{G}_{\mathrm{ee}} & \hat{G}_{\mathrm{eh}} \\ \hat{G}_{\mathrm{he}} & \hat{G}_{\mathrm{hh}} \end{pmatrix}. \quad (2)$$

1) e-mail: avasenko@hse.ru

Table 1. Symmetry classification of the anomalous Green's function. With respect to the sign change of the energy (or Matsubara frequency) and momentum, the Green's function can be even (E) or odd (O). The spin part can be divided into a singlet (S) or three triplet (T) components. The pairing amplitude, given by the anomalous Green's function, must be completely antisymmetric under the sign change of the energy, momentum, and the exchange of spin components of the electrons making up the Cooper pair. The Pauli principle allows for four different combinations; using a "energy/spin/momentum" notation: ESE, OSO, ETO, and OTE.

Symmetry of the induced pairing	Energy/spin/momentum symmetry		
	$E \to -E$	$\sigma \leftrightarrow \sigma'$	$\mathbf{k} \to -\mathbf{k}$
Even-frequency spin-singlet even-parity (ESE)	+	−	+
Odd-frequency spin-singlet odd-parity (OSO)	−	−	−
Even-frequency spin-triplet odd-parity (ETO)	+	+	−
Odd-frequency spin-triplet even-parity (OTE)	−	+	+

The diagonal blocks of the $\check{G}$ matrix describe the propagation of the electrons and holes separately, while the off-diagonal blocks describe the interaction between the electron and hole branches, providing the mixing of the electron and hole degrees of freedom due to Andreev reflections. To characterize the pair potential induced in topological surface we have thus to consider the off-diagonal part of Eq. (2), i.e. the anomalous Green's function. Since $\hat{G}_{\mathrm{eh}}$ and $\hat{G}_{\mathrm{he}}$ are related by complex conjugation it is sufficient to consider one of these matrices.

Expanding $\hat{G}_{\mathrm{eh}}$ in Pauli matrices (where $\hat{\sigma}_0$ is a unitary 2×2 matrix) we can write, $\hat{G}_{\mathrm{eh}} = \mathrm{i}\big(f_0\hat{\sigma}_0 + f_x\hat{\sigma}_x + f_y\hat{\sigma}_y + f_z\hat{\sigma}_z\big)\hat{\sigma}_y$, where f_0 is the spin-singlet component $(\uparrow\downarrow - \downarrow\uparrow)$, f_x and f_y are the combinations of equal spin triplet components, $(\uparrow\uparrow - \downarrow\downarrow)$ and $(\uparrow\uparrow + \downarrow\downarrow)$, correspondingly, while f_z is the hetero-spin triplet component, $(\uparrow\downarrow + \downarrow\uparrow)$. We have shown that the spin-singlet f_0 consists of the ESE and OSO components. We notice that for the OSO pairing realization both nonzero warping and nonzero exchange field should be present in our system. The equal-spin triplet combinations f_x and f_y both consist of the ETO and OTE components. The OTE pairing realization in possible only at $M \neq 0$ or $\lambda \neq 0$. Finally, the hetero-spin triplet component f_z also consists of the ETO and OTE components. In the absence of the hexagonal warping only the OTE pairing remains, but it also disappears at zero magnetic moment.

Based on symmetry arguments we would like to formulate a hypothesis of a possible effect, accessible for direct experimental observation. Let us consider the two-dimensional (2D) S/FI junction formed on the topological insulator surface in x-y plane (the S/FI boundary is located at $x = 0$ along the y-axis). The ferromagnetic insulator layer lies in $x < 0$ half-plane, while the superconductor layer in $x > 0$ half-plane. As above, we consider the exchange field pointing out of the plane in z-direction. Then the Hamiltonian of a TI warped surface state in the presence of an exchange field M can be written as $\hat{H}_M = \hat{H}(\mathbf{k}) + \hat{\sigma}_z M$, where $\hat{H}(\mathbf{k})$ is determined above. Let us project this Hamiltonian on the S/FI boundary, i.e. on the y-axis. Then the effective one-dimensional Hamiltonian for electronic states at the S/FI boundary will look like $\hat{H}_{\mathrm{eff}}(k_y) = -\mu - vk_y\hat{\sigma}_x + \hat{\sigma}_z\lambda k_y^3\cos(3\theta) + \hat{\sigma}_z M$. From the viewpoint of the time reversal and spatial symmetries it is equivalent to the following one-dimensional Hamiltonian of a topological nano-wire, which was recently considered in [5], $\hat{H}_{\mathrm{wire}}(k_y) = -\mu + \alpha k_y\hat{\sigma}_y + \mathbf{M}\hat{\boldsymbol{\sigma}}$, where $\mathbf{M}\hat{\boldsymbol{\sigma}} = M_x\hat{\sigma}_x + M_y\hat{\sigma}_y + M_z\hat{\sigma}_z$, and α is some constant ($M_i \neq 0$, $i = x, y, z$). It was recently shown in [5] that a Josephson junction through such nano-wire will be characterized by spontaneous supercurrent at zero phase difference. In the aforementioned 2D structure it will correspond to the spontaneous supercurrent along the S/FI boundary. It is important to mention that the supercurrent appears only in the model with the hexagonal warping effect.

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