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Odd-frequency superconductivity induced in topological insulators with and without hexagonal warping

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Abstract.   We study the effect of the Fermi surface anisotropy on the odd-frequency spin-triplet pairing component of the induced pair potential. We consider a superconductor/ferromagnetic insulator (S/FI) hybrid structure formed on the 3D topological insulator (TI) surface. In this case three ingredients insure the possibility of the odd-frequency pairing: 1) the topological surface states, 2) the induced pair potential, and 3) the magnetic moment of a nearby ferromagnetic insulator. We take into account the strong anisotropy of the Dirac cone in topological insulators when the chemical potential lies well above the Dirac cone and its constant energy contour has a snowflake shape. Within this model, we propose that the S/FI boundary should be properly aligned with respect to the snowflake constant energy contour to have an odd-frequency symmetry of the corresponding pairing component and to insure the Majorana bound state at the S/FI boundary. For arbitrary orientation of the boundary the Majorana bound state is absent. This provides a selection rule to the realization of Majorana modes in S/FI hybrid structures, formed on the topological insulator surface.

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1. Introduction

Three-dimensional topological insulators (3D TI) represent a recently discovered new state of matter [1, 2, 3, 4, 5]. Their hallmark is the formation of conducting surface states with the Dirac dispersion relation (similar to graphene), whereas the bulk states are gapped. Recently a lot of interest has been attracted to the physics of hybrid structures involving topological insulators and other materials, for example new electronic states have been predicted to appear in TI contacts to ferromagnets and superconductors, such as a magnetic monopole [6] and a Majorana fermion (MF) [7, 8, 9, 10, 11]. A MF has been a primary focus of many extensive studies, since it was proposed as a building block of a topological qubit, that is robust against local decoherence [12].

When the topological insulator is placed in the electrical contact with the superconductor (S), the superconducting pair correlations penetrate into the topological state due to the proximity effect [13, 14]. Its key mechanism is the Andreev reflection process, which provides the possibility for converting single electron states from a topological insulator to Cooper pairs in the superconducting condensate [15]. Recently the S/TI proximity effect was studied by many authors and the formation of an exotic pair potential with the so called odd-frequency spin-triplet pairing component in the TI surface was predicted in some particular cases, for example in the presence of the external magnetic field [16, 17, 18, 19, 20, 21, 22, 23].

In accordance with the Pauli principle, the total wave function of a pair of fermions should be asymmetric and can be described by the product of an orbital (or parity), spin and energy (or Matsubara frequency) term [24]. Even-frequency pairing means that a function is even in energy. If we consider singlet (which is an odd function under spin permutation) s- or d-wave (orbitally symmetric) pairing, the pairing wave function should be even in momentum in order for the wave function to be antisymmetric when the pairing is even in energy. This is the so called even-frequency spin-singlet even-parity (ESE) pairing symmetry class. For p-wave triplet pairing the pairing wave function should be odd in the momentum. This symmetry class is referred to as even-frequency spin-triplet odd-parity (ETO) pairing.

However, the so-called odd-frequency pairing states when the pair amplitude is an odd function of energy can also exist. It was first proposed by Berezinskii in the context of ^{3}He [25]. Then, the odd-frequency spin-singlet odd-parity (OSO) and the odd-frequency spin-triplet even-parity (OTE) pairing states are allowed by the Pauli principle. The OSO pairing is quite generally induced near the normal metal/ superconductor interface during the formation of the Andreev bound states [26, 27, 28]. Recently it was shown, that in S/TI heterostructures another type of an odd-frequency pairing is induced in the presence of the external magnetic field, perpendicular to the topological insulator surface - the OTE pairing state [16, 17, 18, 19, 20, 21, 22, 23]. It was shown by Asano and Tanaka that in a one-dimensional nano-wire, proximity coupled to a topological superconductor, the OTE pairing and the Majorana fermion are "two sides of a same coin" [16]. It was also argued that similar assumption is valid for two-dimensional topological surface states of a three-dimensional topological insulator in proximity with an s-wave superconductor [18, 19, 20, 21, 22]. We note here that the symmetry of the induced pair potential in S/TI structures in the diffusive case was studied in [29, 30].

A Majorana fermion is a topological state that is its own anti-particle, in striking contrast to any known fermion so far [9]. Generally, in solid state physics, electronic transport can either be described in terms of electrons or in terms of holes. The electron and hole excitations in the superconductor play the role of particle and antiparticle. Electrons (filled states above the chemical potential) and holes (empty states below the chemical potential) have opposite spin and charge, but the charge difference of $2e$ can be absorbed as a Cooper pair in the s-wave superconducting condensate. In order for a Majorana fermion to exist, it would have to be simultaneously half-electron and half-hole and electrically neutral. Therefore, the zero energy is a likely place to look for a Majorana fermion. Experimentalists have already reported signatures of the Majorana zero-energy mode, where zero-bias conductance peaks are the main features observed in this context [31, 32, 33, 34]. Signatures of Majorana zero modes were also observed in the Josephson effect in HgTe-based junctions [35, 36], in ferromagnetic atomic chains formed on a superconductor [37], and in a semiconductor Coulomb island in proximity with a superconductor [38]. Impressive number of theoretical studies of electron transport in different hybrid devices containing Majorana fermions was published in recent years [39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56].

Majorana fermions in superconductor/ topological insulator (S/TI) hybrid structures have been first predicted by Fu and Kane [39] as zero energy states at the site of a vortex, induced by the magnetic field on the surface of the

topological insulator in proximity with a superconductor. A MF was also predicted to occur if the externally applied magnetic field is replaced by the magnetic moment of a nearby ferromagnetic insulator (FI). In the latter case, the Majorana fermion turns out to be a one-dimensional linearly dispersing mode along the S/FI boundary, when a S/FI junction is formed on the topological insulator surface [40].

In this work we study the interplay between topological order and superconducting correlations performing a symmetry analysis of the induced pair potential based on the anomalous Green function and analyze the conditions of possible realization of the Majorana mode in a hybrid structure, where a S/FI junction is formed on the topological surface as shown in Fig. 2(a) [18, 40]. We take into account the hexagonal warping effect, which was never considered previously in this connection, for example in Ref. [18]. Since the Majorana fermion and the odd-frequency spin-triplet even-parity (OTE) pairing are related to each other it is important to study the effect of the hexagonal warping on the OTE pairing component realization of the proximity effect. In the end of the paper we make some predictions about the MF realization in the structure under consideration, based on the symmetry arguments.
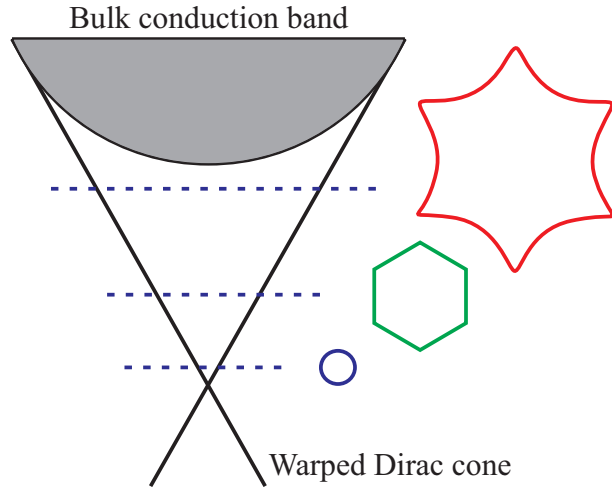
2. Hexagonal warping

The aforementioned studies of the proximity effect and the Majorana bound states on the surface of a 3D topological insulator were performed within the simplest model, when the energy dispersion was described with an isotropic Dirac cone. Within the $k \cdot p$ theory a 2×2 Hamiltonian of surface states in this model to the lowest order in k reads $-\mu + v(k_x \hat{\sigma}_x + k_y \hat{\sigma}_y)$ [so called Dirac-type Hamiltonian]. 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 ($j = x, y, z$). It is also possible to use a Bychkov-Rashba term [57] in the Hamiltonian of a topological insulator,

$$\hat{H}_0(\mathbf{k}) = -\mu + v(k_x \hat{\sigma}_y - k_y \hat{\sigma}_x). \tag{1}$$

This gives rise to a different spin-momentum locking on the Fermi surface [3, 4]. Nevertheless, all conclusions on the excitation spectrum are independent of whether one uses the Dirac or Bychkov-Rashba type of the Hamiltonian [58]. However, such isotropic forms of the Hamiltonian are only valid if the chemical potential lies near the Dirac point, while in realistic topological insulators it usually lies well above this point, where the Dirac cone distortion can't be any more neglected.

To develop more realistic theoretical description of the superconducting proximity effect in the topological insulator surface states it is important to take into account the Dirac cone anisotropy. For example, the Fermi surface of Bi_2Te_3 topological insulator observed by angle resolved photoemission spectroscopy (ARPES) is nearly

Figure 1. The hexagonal warped Dirac cone in three-dimensional topological insulators, shown schematically. A set of constant energy contours for different chemical potential positions (shown by dashed blue lines) is presented. Near the Dirac point the constant energy contour is almost circular, evolving to hexagonal with increasing energy, and then to snowflake near the bulk conduction band.

a hexagon, having snowflake-like shape: it has relatively sharp tips extending along six directions and curves inward in between [59, 60, 61]. Moreover, the shape of constant energy contour is energy-dependent, evolving from a snowflake to a hexagon and then to a circle near the Dirac point, see Fig. 1. Later same anisotropy was found in Bi_2Se_3 [62, 63], $Pb(Bi,Sb)_2Te_4$[64] and other topological insulator materials [65].

Recently it was realized that the aforementioned simplified Hamiltonian can be extended to higher order terms in the momentum. Namely, Fu found an unconventional hexagonal warping term $\hat{H}_w(\mathbf{k})$ in the surface band structure, which is the counterpart of cubic Dresselhaus spin-orbit coupling in rhombohedral structures [66]. The effective Hamiltonian of surface states then reads,

$$\hat{H}(\mathbf{k}) = \hat{H}_0(\mathbf{k}) + \hat{H}_w(\mathbf{k}), \tag{2}$$

where $\hat{H}_0(\mathbf{k})$ is given by Eq. (1), the hexagonal warping term reads

$$\hat{H}_w(\mathbf{k}) = \frac{\lambda}{2}(k_+^3 + k_-^3)\hat{\sigma}_z, \tag{3}$$

$k_\pm = k_x \pm i k_y$, and λ is the hexagonal warping strength. The Hamiltonian in Eq. (2) describes perfectly the warped Dirac cone as schematically shown in Fig. 1. It is the consequence of the rhombohedral crystal structure symmetry, typical to three-dimensional topological insulators. Representative values for the material parameters v and λ can be inferred from ARPES (see for instance [65] and references therein). We stress here that the term in Eq. (3) is different from the trigonal warping term in graphene [66, 67].

The warping term, Eq. (3), breaks the rotational symmetry of the Dirac cone. Moreover, it is an odd-parity term, since it is odd under transformation $\mathbf{k} \rightarrow$

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$-\mathbf{k}$. It is then obvious that addition of this term may dramatically change the physical properties of topological insulator surface states. The consequences of warping on magnetic [66, 68, 69] and transport properties [70, 71] of topological insulators have been discussed extensively in the literature. Recently the magnetic order on a topological insulator surface with hexagonal warping and proximity-induced superconductivity was also studied in [72].

3. Model and basic equations

We consider an s-wave superconductor/ ferromagnetic insulator (S/FI) junction formed on the surface of a three-dimensional topological insulator in the *x-y* plane, see Fig. 2(a), which was previously considered in [18]. The S/FI boundary is perpendicular to the *x*-direction, so that the FI layer lies in $x > 0$ half-plane, while the S layer in $x < 0$ half-plane. Since the superconducting correlations extend in the lateral direction on the scale of superconducting coherence length, we can consider both the superconducting pair potential and the magnetic moment in the effective **k**-dependent Hamiltonian [18], describing the TI surface states in vicinity of the S/FI boundary (we use "check" for 4×4 and "hat" for 2×2 matrices),

$$\check{H}_S(\mathbf{k}) = \begin{pmatrix} \hat{H}(\mathbf{k}) + M\hat{\sigma}_z & \hat{\Delta} \\ -\hat{\Delta} & -\hat{H}^*(-\mathbf{k}) - M\hat{\sigma}_z \end{pmatrix}. \quad (4)$$

Here $\hat{\Delta} = i\hat{\sigma}_y\Delta$, where Δ is the superconducting pair potential, induced in the topological insulator surface due to the proximity effect, and M is the spin-splitting (exchange) field of the ferromagnetic insulator, which we consider to be perpendicular to the topological surface, i.e. along the *z*-axis.

In order to determine the pairing relations for the topological surface states near the S/F boundary we start with the following equation,

$$[E - \check{H}_S(\mathbf{k})]\check{G} = \check{I}, \quad (5)$$

where $\check{G}$ is the Green's function of the topological states in vicinity of the S/FI boundary, $\check{I}$ is the unitary 4×4 matrix, and E is the quasiparticle energy counted from the chemical potential.

Introducing the crystallographic angle θ which is the azimuth angle of momentum **k** with respect to the *x*-axis, so that $k_x = k\cos(\theta)$, $k_y = k\sin(\theta)$, $k = |\mathbf{k}|$, we can write the matrix in the left hand side of Eq. (5) in the following form,

$$[E - \check{H}_S(\mathbf{k})] \equiv \begin{pmatrix} \hat{h}_+ & -\hat{\Delta} \\ \hat{\Delta} & \hat{h}_- \end{pmatrix}, \quad (6)$$

where the matrices $\hat{h}_\pm$ are given by,

$$\begin{pmatrix} \varepsilon_\mp \pm \mu - \lambda k^3 \cos(3\theta) & \pm ivke^{\mp i\theta} \\ \mp ivke^{\pm i\theta} & \varepsilon_\pm \pm \mu + \lambda k^3 \cos(3\theta) \end{pmatrix}, \quad (7)$$

and $\varepsilon_\pm = E \pm M$. The $e^{\pm i\theta}$ factors reflect the chiral odd-parity (p-wave) character of a topological insulator surface in proximity with an s-wave superconductor.

By taking the inverse of the matrix equation (5) we can obtain the Green's function $\check{G}$ expressed as

$$\check{G} = \begin{pmatrix} \hat{G}_{ee} & \hat{G}_{eh} \\ \hat{G}_{he} & \hat{G}_{hh} \end{pmatrix}. \quad (8)$$

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 superconducting pairing correlations induced in the topological surface states we have thus to consider the the off-diagonal part of Eq. (8), i.e. the anomalous Green's function. Since $\hat{G}_{eh}$ and $\hat{G}_{he}$ are related by complex conjugation it is sufficient to consider one of these matrices, given by the following expression,

$$\hat{G}_{eh} = (\hat{\Delta} + \hat{h}_-\hat{\Delta}^{-1}\hat{h}_+)^{-1}. \quad (9)$$

4. Surface states without warping

In this section we reproduce some of the results from [18], rewriting all important equations in our notations for comparison with formulae in the next section (where we take into account the hexagonal warping effect). For now, we focus on the hybrid structure in Fig. 2(a), and assume surface topological insulator states without hexagonal warping, i.e. $\lambda = 0$ in Eq. (3). In this case $\hat{H}(\mathbf{k}) = \hat{H}_0(\mathbf{k})$ in Eq. (2).

Expanding $\hat{G}_{eh}$ in Pauli matrices (where $\hat{\sigma}_0$ is a unitary 2×2 matrix) we obtain [73],

$$\hat{G}_{eh} = i(f_0\hat{\sigma}_0 + f_x\hat{\sigma}_x + f_y\hat{\sigma}_y + f_z\hat{\sigma}_z)\hat{\sigma}_y, \quad (10)$$

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, $(\uparrow\downarrow + \downarrow\uparrow)$ [22]. We can write these pairing wave functions explicitly as [18],

$$f_0 = \frac{\Delta}{Z}\left(E^2 - v^2k^2 - B\right), \quad (11a)$$

$$f_x = \frac{2\Delta}{Z}kv[\mu\sin(\theta) + iM\cos(\theta)], \quad (11b)$$

$$f_y = -\frac{2\Delta}{Z}kv[\mu\cos(\theta) - iM\sin(\theta)], \quad (11c)$$

$$f_z = \frac{2\Delta}{Z}EM, \quad (11d)$$

where we have used the following notations

$$Z = -4k^2v^2(\mu^2 - M^2) - 4E^2M^2 + (E^2 - v^2k^2 - B)^2, \quad (12a)$$

$$B = \mu^2 + \Delta^2 - M^2. \quad (12b)$$

We note that $Z(\mathbf{k}, E)$ in Eq. (12a) is an even function in energy and momentum (even-frequency and even-parity function). The spin-singlet component f_0 belongs to the even-frequency spin-singlet even-parity class (ESE). The two combinations of equal spin components (f_x and f_y) belong to the even-frequency spin-triplet odd-parity class

(ETO). Finally, the hetero-spin triplet f_z belongs to the odd-frequency spin-triplet even-parity class (OTE) [26]. Its presence indicates the possibility of a Majorana fermion realization, according to recent studies [16, 17, 18, 19, 20, 21, 22, 23].

It follows from Eq. (11d) that the f_z pairing function appears only when three ingredients 1) the topological surface states, 2) the superconducting pair potential Δ due to the proximity effect, and 3) the nonzero exchange field M in the z-axis direction, are brought together (which happens in the vicinity of the S/FI boundary in the structure under consideration). When any of these ingredients is missing the anomalous Green's function loses the odd-frequency pairing symmetry. It was also shown that combining these ingredients together is necessary to have the Majorana fermion realization [39, 40]. However, the mere presence of the OTE pairing function f_z still does not mean that a Majorana zero-energy mode exists, because the zero energy mode is not yet fully localized. In Sec. 6 we discuss the localization problem of the Majorana fermion when f_z has pure OTE symmetry.

5. Warped surface states

If we now 'switch on' the hexagonal warping, so that $\lambda \neq 0$ in Eq. (3), the pairing wave functions in Eq. (10) read,

$$f_0 = \frac{\Delta}{Z_+}\left(E^2 - E_S^2 - B\right), \tag{13a}$$

$$f_x = \frac{2\Delta}{Z_+}kv\left[\mu\sin(\theta) + iM\cos(\theta)\right], \tag{13b}$$

$$f_y = -\frac{2\Delta}{Z_+}kv\left[\mu\cos(\theta) - iM\sin(\theta)\right], \tag{13c}$$

$$f_z = \frac{2\Delta}{Z_+}\left[EM - \mu\lambda k^3\cos(3\theta)\right]. \tag{13d}$$

In Eq. (13a) E_S is given by the following relation,

$$E_S = \sqrt{v^2k^2 + \lambda^2k^6\cos^2(3\theta)}. \tag{14}$$

It determines the surface band dispersion of the Hamiltonian in Eq. (2), i.e. the energy dispersion relation for the bare topological insulator surface, taking into account the hexagonal warping effect [66],

$$E_{1,2} = -\mu \pm E_S. \tag{15}$$

Here $E_{1,2}$ denote the energy of upper and lower band.

In Eqs. (5) the Z_+ function is given by,

$$Z_{\pm}(\mathbf{k}, E) = -4k^2v^2(\mu^2 - M^2) + (E^2 - M^2)^2 + E_-^2 E_+^2$$
$$- E_{\mp}^2(E - M)^2 - E_{\pm}^2(E + M)^2, \tag{16}$$

where we used the following notations,

$$E_{\pm} = \sqrt{v^2k^2 + \Delta^2 + [\mu \mp \lambda k^3\cos(3\theta)]^2}. \tag{17}$$

Using the equalities

$$Z_{\pm}(\mathbf{k}, E) = Z_{\pm}(-\mathbf{k}, -E), \tag{18a}$$

$$Z_{\pm}(-\mathbf{k}, E) = Z_{\pm}(\mathbf{k}, -E) = Z_{\mp}(\mathbf{k}, E). \tag{18b}$$

we can introduce the functions

$$F_{\text{even}} = \Delta/Z_+ + \Delta/Z_-, \tag{19a}$$

$$F_{\text{odd}} = \Delta/Z_+ - \Delta/Z_-, \tag{19b}$$

where Z_- is defined in Eq. (16). It is easy to see that F_{even} is even in energy and momentum, while F_{odd} is odd in both arguments. We notice that changing the momentum sign $\mathbf{k} \to -\mathbf{k}$ is equivalent to $\theta \to \theta + \pi$ rotation.

In our spin basis the spin-triplet f_x and f_y pairing functions are the combinations of equal spin components, $(\uparrow\uparrow - \downarrow\downarrow)$ and $(\uparrow\uparrow + \downarrow\downarrow)$, correspondingly, while the function f_z is the hetero-spin triplet component, $(\uparrow\downarrow + \downarrow\uparrow)$. Therefore only f_z is providing the spin-mixing, required for the realization of an electron-hole superposition due to Andreev reflections at the s-wave superconductor interface, which can form a Majorana fermion under certain conditions [9]. It can be written in the following symmetrized form $f_z = f_z^- + f_z^+$, where

$$f_z^- = EMF_{\text{even}} - \mu\lambda k^3\cos(3\theta)F_{\text{odd}}, \tag{20a}$$

$$f_z^+ = EMF_{\text{odd}} - \mu\lambda k^3\cos(3\theta)F_{\text{even}}. \tag{20b}$$

If we take into account the hexagonal warping, the f_z component is no more odd in energy, as in the previous section 4, since the f_z^+ term is even in energy for any chosen $\mathbf{k}$ direction, see Eq. (20b). The z-component of the anomalous Green's function became odd in energy only at the following six values of the angle θ,

$$\theta_n = \pi/6 + \pi n/3, \tag{21}$$

which correspond to the six tips of the snowflake constant energy contour, shown in Fig. 2(b) (n is an integer number). At these values of θ the $\cos(3\theta)$ term tends to zero. In the same time $F_{\text{odd}} = 0$ since $E_+ = E_- = \sqrt{v^2k^2 + \Delta^2 + \mu^2}$ in Eq. (17) and $Z_+ = Z_- \equiv Z$. As a result at $\theta = \theta_n$ the hexagonal warping effectively disappears and the f_z pairing function is given by Eq. (11d) in Sec. 4. So, at $\theta = \theta_n$ we have a possibility of the Majorana fermion realization.

6. Majorana modes

Let us now consider six lines $\theta = \theta_n$ on the TI surface, where the topological surface spectrum is given by the following relation [which can be obtained by diagonalization of the Hamiltonian in Eq. (4)],
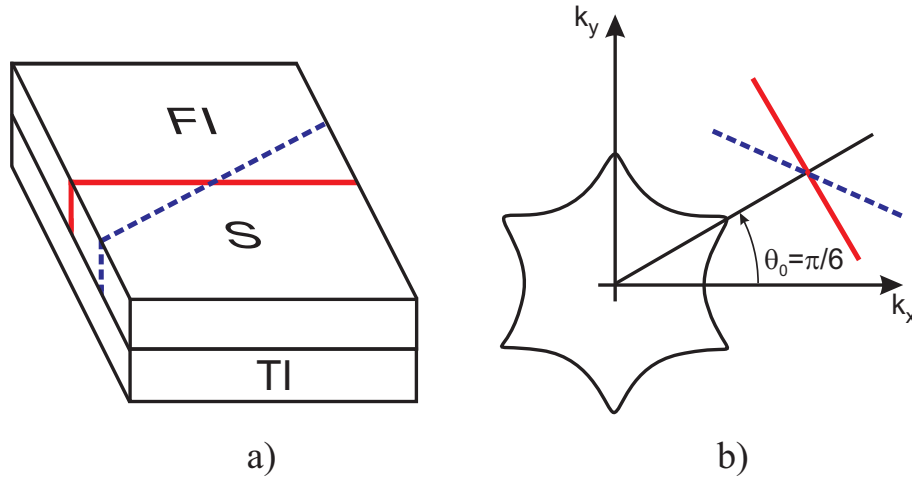
$$E_{1,2,3,4} = (\pm)(\mp 1) \times \tag{22}$$
$$\sqrt{\mu^2 + \Delta^2 + v^2k^2 + M^2 \pm 2\sqrt{\mu^2v^2k^2 + M^2[\mu^2 + \Delta^2]}}.$$

In this expression we need to take all possible combinations of $\pm$ signs to get four energy bands. In the limit of $\mu \gg \Delta$, which is often the case, this can in good approximation be written as [18]

$$E_{1,2,3,4} = \pm(\mp)\mu \pm \sqrt{v^2k^2 + M^2}. \tag{23}$$

As was mentioned in Sec. 4, in order to have a zero-energy Majorana mode for $\theta = \theta_n$, it needs to be localized

Figure 2. (a) Schematic illustration of the structure under consideration: superconductor/ ferromagnetic insulator (S/FI) junction formed on the surface of a three-dimensional topological insulator, TI. The *x*-axis is chosen perpendicular to the S/FI boundary. Two possible S/FI boundaries are shown by solid red and dashed blue lines as explained in Fig. 2(b). (b) Two possible alignments of the S/FI boundary with respect to the snowflake constant energy contour of the warped Dirac cone. The one, shown by solid red line, is favorable for the Majorana bound state realization, see details in the text. There are overall six favorable alignments at θ_n values, corresponding to the six tips of the snowflake contour. The favorable alignment should be perpendicular to the line, connecting the tip and the center of the snowflake contour. Arbitrary boundary alignments, for example the one, shown by dashed blue line, are unfavorable and do not host the Majorana bound states.

both at the superconducting side and at the side of the ferromagnetic insulator. At the superconducting side it happens due to the superconducting gap. At the FI side the exchange field M has to be large enough so that the chemical potential is inside the gap [18], $M > \sqrt{\Delta^2 + \mu^2}$, or just $M > \mu$ if $\mu \gg \Delta$. Then the zero-energy mode is fully localized. As was shown in [18] the midgap Andreev bound state became the Majorana zero mode only when the incident electron and the Andreev-reflected hole trajectories are perpendicular to the S/FI boundary ($k_y \sim 0$). As follows from the above arguments to insure the MF existence the S/FI boundary should be aligned perpendicular to the line $\theta = \theta_n$.

In Fig. 2(b) we show the alignment of the S/FI boundary (shown by solid red line) which insures the Majorana zero energy mode existence in particular case $\theta_0 = \pi/6$. Generally, the boundary should be perpendicular to the line $\theta = \theta_n$ in the topological surface plane and totally six favorable alignments are possible. The expressions for the Majorana zero modes given in [18] hold in our case for $\theta = \theta_n$. In the vicinity of $\theta = \theta_n$ the bound state energy is $E = -\Delta \sin(\theta - \theta_n)$ and goes to zero at $\theta = \theta_n$.

For $\theta \neq \theta_n$, the surface bound states dispersion relations for finite λ become very cumbersome and we do not present them here. But, importantly, based on the assumption on direct correspondence between the hetero-spin pure OTE component and the Majorana fermion in 2D topological surface [18], one can provide the following general symmetry-based argument. Since the triplet component f_z of the anomalous Green's function is neither odd nor even in energy in this case [see Eqs. (20a)], no zero-energy Majorana bound states will be formed for any

alignment of the S/FI boundary except six aforementioned. The example of such unfavorable alignment is shown in Fig. 2(b) by a blue dashed line. This may provide a selection rule to the realization of Majorana modes in S/FI hybrid structures, formed on the topological insulator surface. Recently another type of a selection rule for the MF realization was established in [74].

7. Conclusion

In conclusion, we have theoretically discussed the proximity effect in three-dimensional topological insulators with warped surface state, in the presence of a magnetic moment, perpendicular to the TI surface. For this we have considered a superconductor/ ferromagnetic insulator heterostructure, formed on the surface of a topological insulator, see Fig. 2(a).

We have discussed the hetero-spin odd-frequency spin-triplet even-parity (OTE) pairing, induced in the warped TI surface state by proximity with a superconductor and its relation with the Majorana fermion state. In a one-dimensional nano-wire the pure OTE pairing and the Majorana zero mode "are one and the same thing" [16, 17]. It was also argued that same statement is valid in the two-dimensional case of a 3D topological insulator surface [18]. Then the Majorana fermion realization is sensible to the orientation of the S/FI boundary with respect to the snowflake constant energy contour of the warped Dirac cone. The favorable alignment should be perpendicular to the line, connecting the snowflake tip and the center of the snowflake contour. Arbitrary boundary alignments are unfavorable and do not host the Majorana bound states.

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This may provide a selection rule to the realization of Majorana modes in S/FI hybrid structures, formed on the topological insulator surface.

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