Majorana modes in three-dimensional topological insulators with warped surface state

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HEXAGONAL WARPING IN TOPOLOGICAL INSULATORS

Many theoretical predictions about magnetic and transport properties of topological insulators were made on the basis of a simplified model, when the topological surface states were described with an isotropic Dirac cone. However, such isotropic models 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.

For example, the Fermi surface of Bi_2Te_3 topological insulator observed by angle resolved photoemission spectroscopy (ARPES) is nearly a hexagon, having snowflake-like shape: it has relatively sharp tips extending along six directions and curves inward in between [1,2]. 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.

Recently it was realized that without violation of the symmetry the simplified Hamiltonian can be extended to higher order terms in the momentum. Namely, Fu found an unconventional hexagonal warping term in the surface band structure [3]. The effective Hamiltonian of surface states then reads,

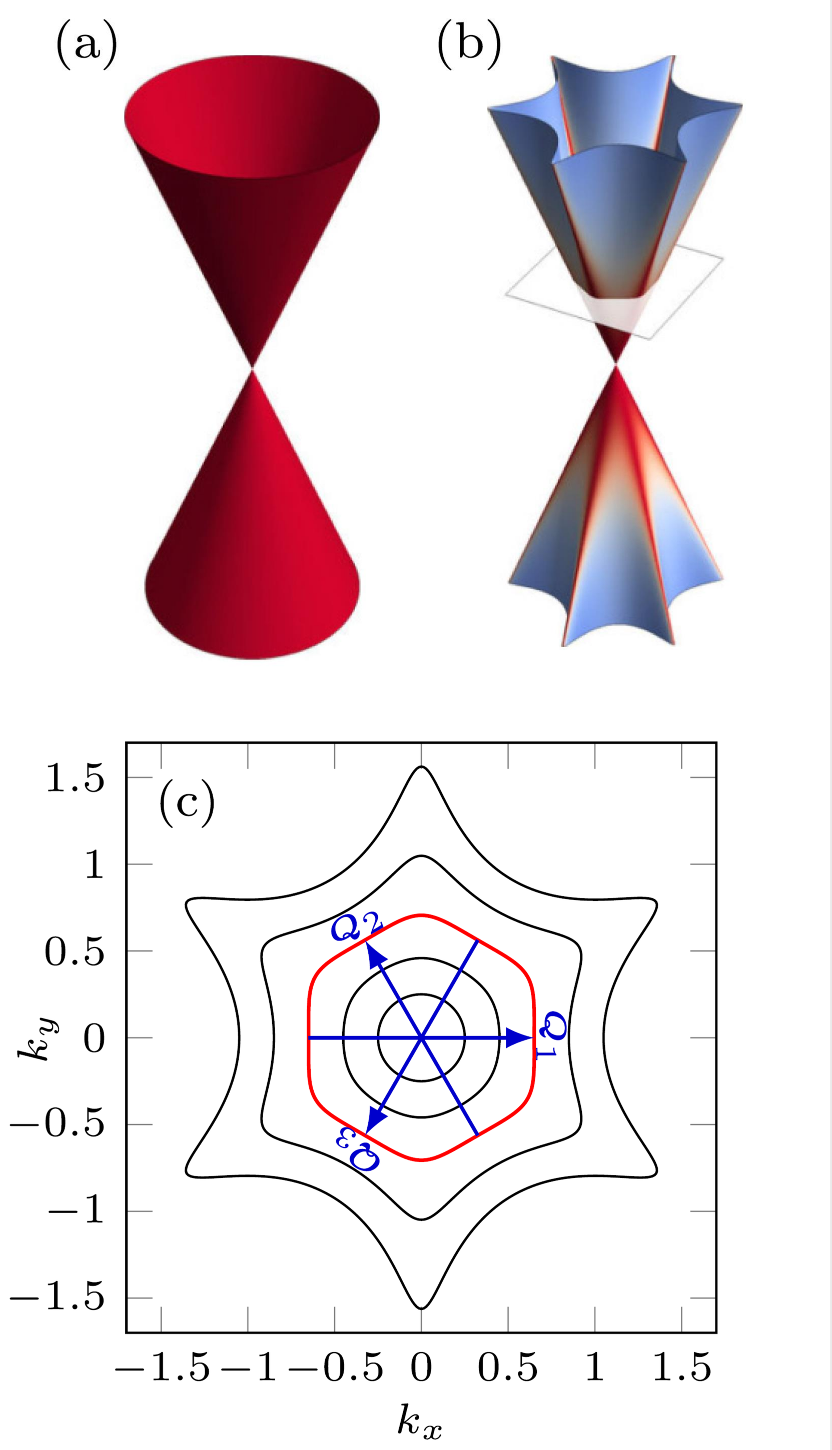
$$\hat{H}(\mathbf{k}) = -\mu + v(k_x\hat{\sigma}_y - k_y\hat{\sigma}_x) + \hat{H}_{\mathrm{w}}(\mathbf{k})$$

where the hexagonal warping term is given by

$$\hat{H}_{\mathrm{w}}(\mathbf{k}) = \frac{\lambda}{2}(k_+^3 + k_-^3)\hat{\sigma}_z$$

Here $k_\pm = k_x \pm i k_y$, $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are the Pauli matrices in spin space, **k** denotes in-plane quasiparticle momentum, μ is a chemical potential, v is a Fermi velocity, and λ is the hexagonal warping strength.

Fig.1 to the right is taken from Ref.4.



MAJORANA FERMION

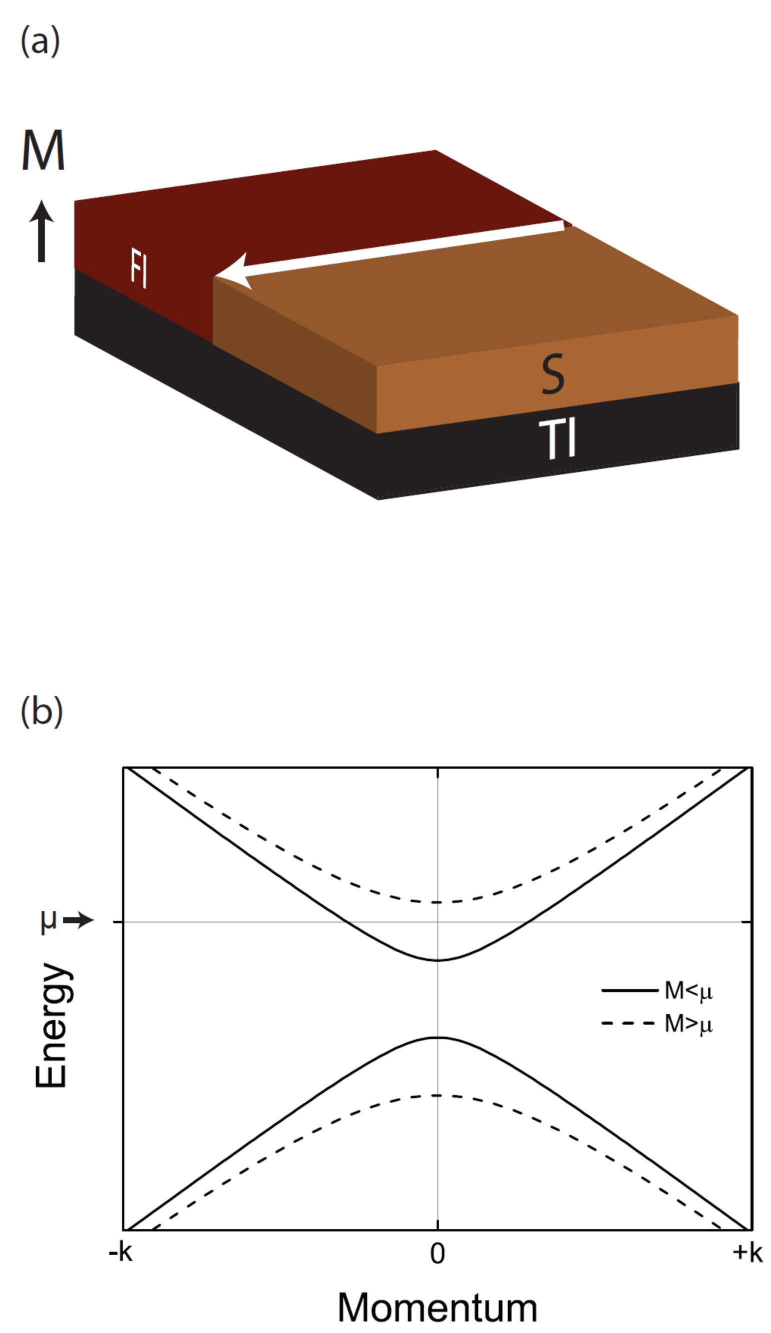
A Majorana fermion is a topological state that is its own anti-particle, in striking contrast to any known fermion so far. Generally, in solid state physics, electronic transport can either be described in terms of electrons or in terms of holes. In order for a Majorana fermion to exist, it would have 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 [5,6].

Majorana fermions in superconductor/ topological insulator (S/TI) hybrid structures have been first predicted by Fu and Kane [7] 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 Majorana fermion was also predicted to occur if the externally applied magnetic field is replaced by the magnetic moment of a nearby ferromagnetic insulator (FI) [8]. 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. The ferromagnetic insulator was taken to insure that the current is only going through the surface states.

Fig.2 to the right is taken from Ref.9.

(a) A ferromagnet insulator(FI) can both break time-reversal symmetry and localize the Majorana zero-energy mode in a TI. The location of the Majorana mode is indicated by the white arrow.

(b) The dispersion relation of the topological insulator at the ferromagnet side for a magnetization smaller and larger than the chemical potential. In the former, the chemical potential still lays in the Dirac cone. In the latter, the states around the chemical potential are gapped out and the zero-energy mode is localized at the interface between the superconductor and ferromagnet.



ANOMALOUS GREEN'S FUNCTION SYMMETRY

We present the Hamiltonian for the TI surface states in the vicinity of FI/S boundary and solve the master equation to obtain the Green's function. Here M is the magnetic moment of FI and Δ is the superconducting pair potential.

To characterize the Majorana zero mode we have to consider the off-diagonal part of the Green's function, i.e. the anomalous Green's function. It can be expanded in Pauli matrices [10]. Here τ-matrix acts in Nambu space.

We are interested in the odd-frequency component, since according to many recent studies it is directly related to the Majorana fermion existence [9,11,12,13].

We introduce the angle θ so that

$$k_x = k\cos(\theta),\ k_y = k\sin(\theta)$$

Without warping only f_z belongs to odd-frequency class (OTE, see Fig.3 to the right taken from Ref.12). Here

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

$$Z_\pm(\theta, E) = Z_\pm(\theta+\pi, -E),$$
$$Z_\pm(\theta+\pi, E) = Z_\pm(\theta, -E) = Z_\mp(\theta, E)$$

Introducing the functions $F_{e,o}$ we can write

$$F_{\mathrm{e}} = \Delta/Z_+ + \Delta/Z_-, \quad F_{\mathrm{o}} = \Delta/Z_+ - \Delta/Z_-$$

$$f_z^{\mathrm{oe}} = EMF_{\mathrm{e}} - \mu\lambda k^3\cos(3\theta)F_{\mathrm{o}}$$
$$f_z^{\mathrm{eo}} = EMF_{\mathrm{o}} - \mu\lambda k^3\cos(3\theta)F_{\mathrm{e}}$$

In our spin basis $f_x \propto (\uparrow\uparrow - \downarrow\downarrow),\ f_y \propto (\uparrow\uparrow + \downarrow\downarrow)$

Therefore only $f_z \propto (\uparrow\downarrow + \downarrow\uparrow)$ provides the spin-mixing, required for the Majorana fermion realization.

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

$$\left[E - \check{H}_S(\mathbf{k})\right]\check{G} = \check{1} \qquad \check{G} = \begin{pmatrix} \hat{G}_{\mathrm{ee}} & \hat{G}_{\mathrm{eh}} \\ \hat{G}_{\mathrm{he}} & \hat{G}_{\mathrm{hh}} \end{pmatrix}$$

$$\hat{G}_{\mathrm{eh}} = i\left(f_0\hat{\sigma}_0 + f_x\hat{\sigma}_x + f_y\hat{\sigma}_y + f_z\hat{\sigma}_z\right)\hat{\tau}_y$$

$$f_0 = \frac{\Delta}{Z_+}\left(E^2 + M^2 - \mu^2 - \Delta^2 - E_S^2\right)$$

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

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

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

	$F_{\sigma\sigma'}(\omega,k) = -F_{\sigma'\sigma}(-\omega,-k)$		
	$\omega \to -\omega$	$\sigma \leftrightarrow \sigma'$	$k \to -k$
ESE	+	−	+
OSO	−	−	−
ETO	+	+	−
OTE	−	+	+

MAJORANA FERMION AND WARPING

It was shown previously that odd in energy triplet f_z component is required for the Majorana zero mode existence [11,12,13]. It appears naturally in isotropic models with no warping (λ=0) when finite out-of-plane magnetic field is applied to the structure (or the FI magnetic moment in our consideration) [9].

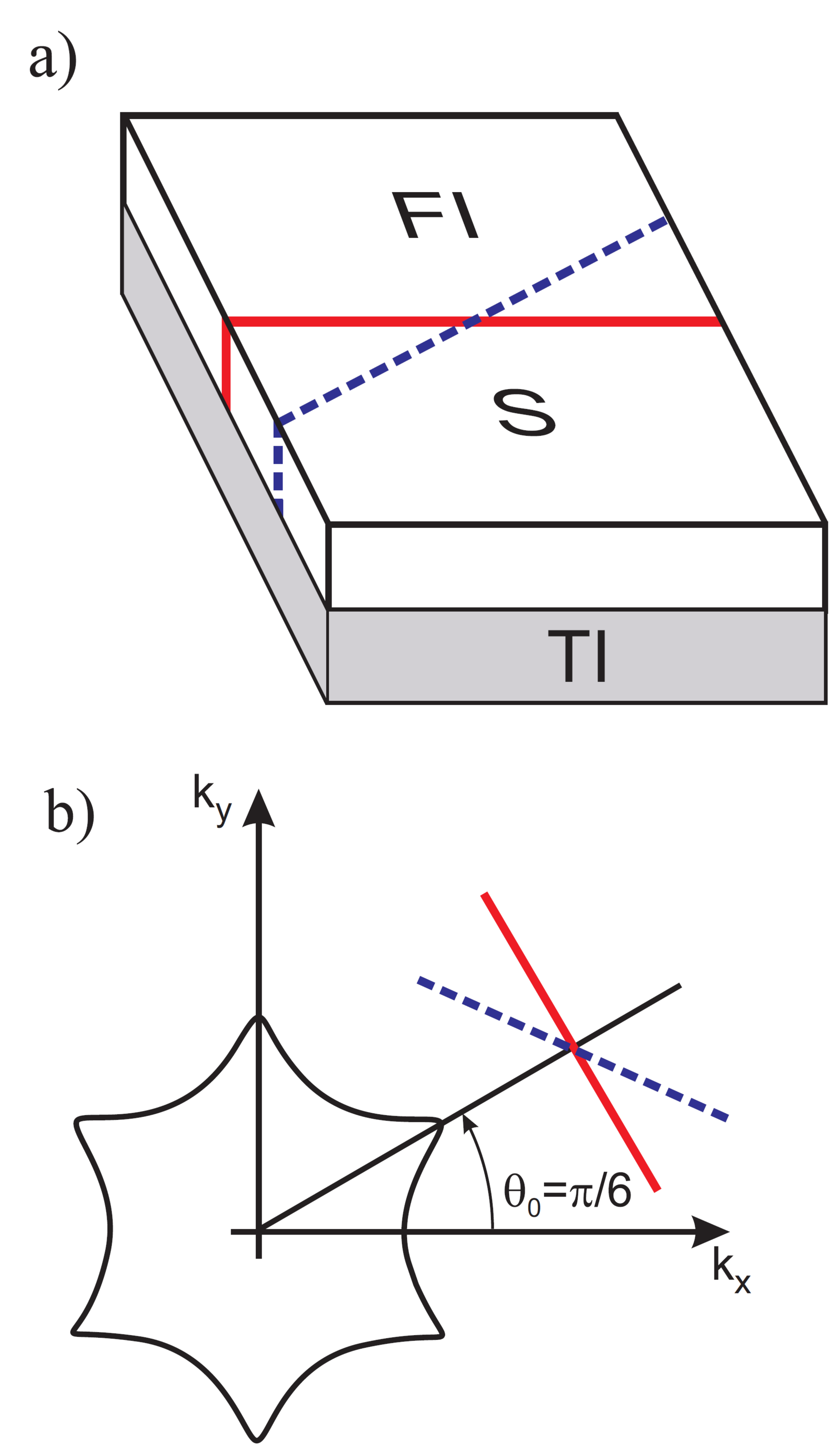
In our model including warping effects, the z-component of the anomalous Green's function became odd in energy only at the following six values of the crystallographic angle θ

$$\theta_n = \pi/6 + \pi n/3$$

which correspond to the six tips of the snowflake constant energy contour. At other values of θ the z-component is neither odd nor even in energy and the Majorana zero energy mode does not exist.

As was shown in Ref.9 the midgap Andreev bound state became the Majorana zero mode only when incident electron and the Andreev-reflected hole trajectories are perpendicular to the S/FI boundary. As follows from the above arguments to insure the MF existence the S/FI boundary should be aligned perpendicular to the line $\theta = \theta_n$.

Fig.4 to the right illustrates the principal result of this work [14]. If one takes the hexagonal warping effects into account the proper alignment of the S/FI boundary with respect to the snowflake constant energy contour of the TI Dirac cone is crucial to obtain the localized Majorana zero-energy mode. This provides a very important selection rule to the realization of Majorana modes in S/FI hybrid structures, from the topological insulator surface. It also gives a guideline for the observation of the Majorana fermion in experiments.



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