



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

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Topological insulator in a nutshell

...a new state of matter that has been predicted and discovered!

- Bulk is insulating; edge (2D)/ surface (3D) a very good conductor.
- Important ingredient: spin-orbit coupling:

opposite force for opposite spins.

- Topological invariant is insensitive to any continuous deformation of Hamiltonian (**topological protection**): disorder, geometry, weak interactions, etc...

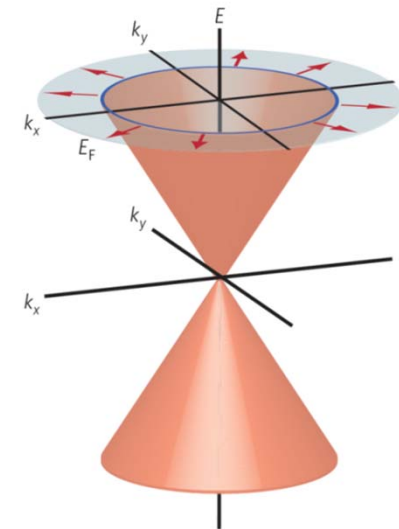
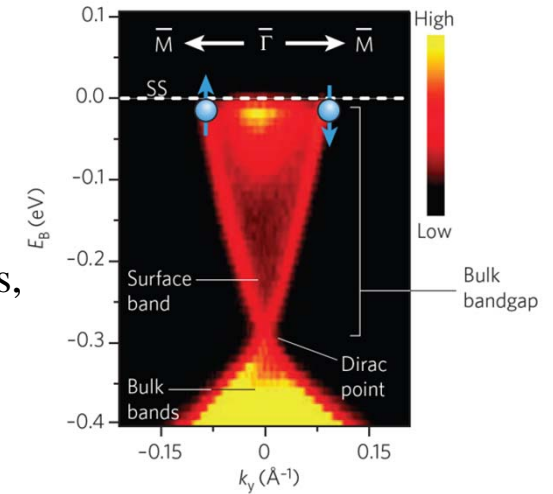
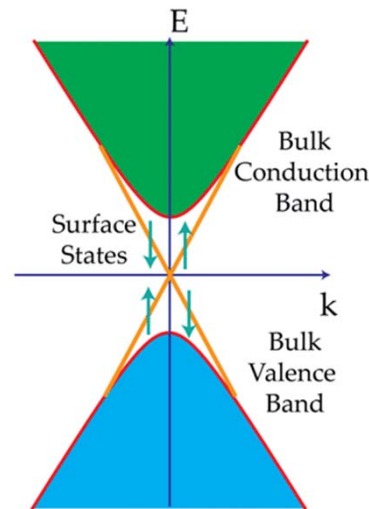
Examples:

- **2D**: HgTe/CdTe; **3D**: Bi₂Se₃, Bi₂Te₃, Sb₂Te₃, TlBiSe₂, Bi₂Te₂Se.



2D

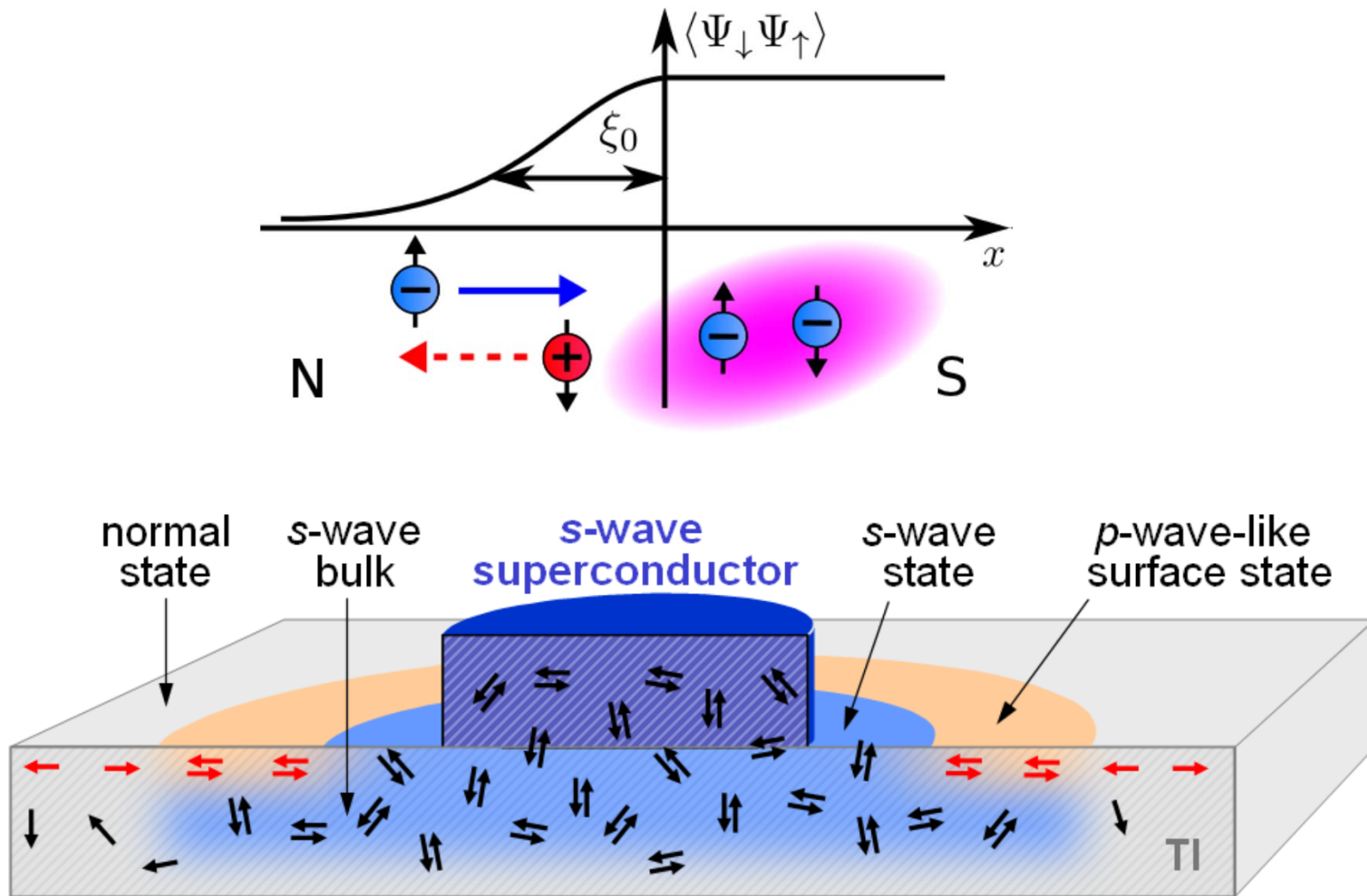
Theo1: C.L. Kane and E.J. Mele, **PRL** 95, 226801 (2005)
Theo2: B.A. Bernevig et al., **Science** 314, 1757 (2006)
Exp: M. König et al., **Science** 318, 766 (2007)



3D

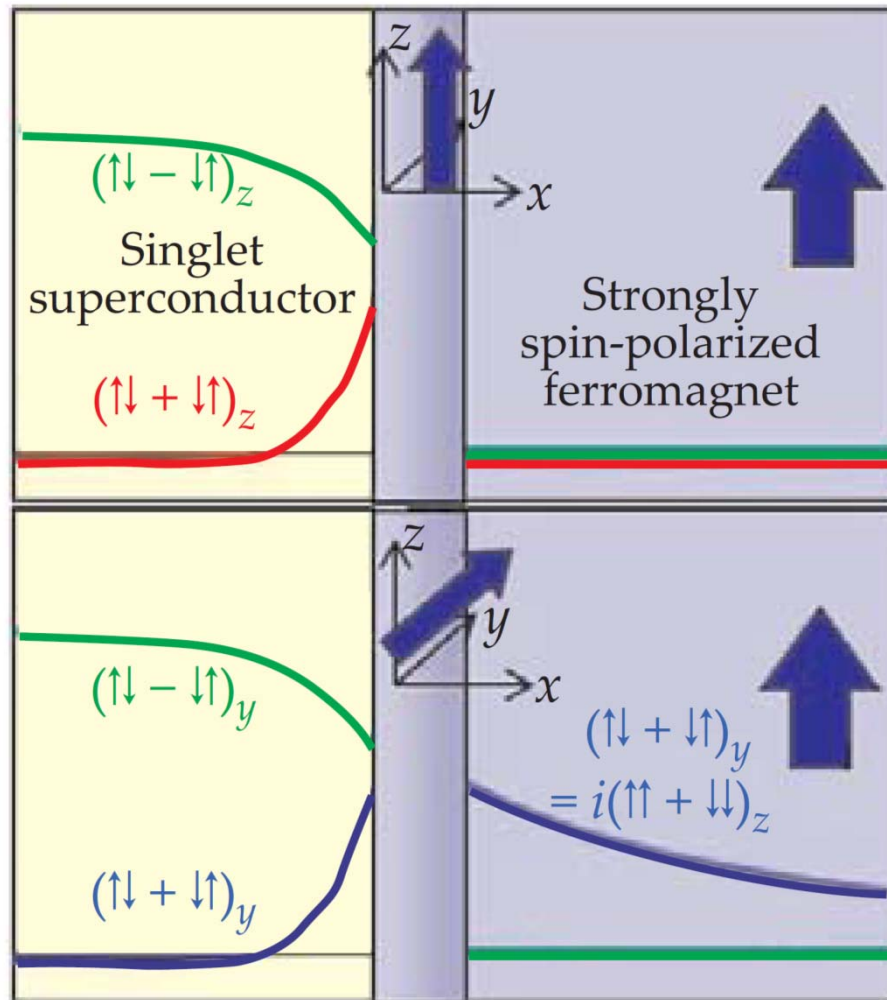
Theo: L. Fu, et al., **PRL** 98, 106803 (2007)
Exp1: Zhang H. et al., **Nat. Phys.** 5, 438 (2009)
Exp3: S. Tokafuji et al., **PRL** 105, 136802 (2010)

Superconductor/ topological insulator proximity effect



J. Shen et al., arXiv:1303.5598 (2013)

Spin-triplet superconductivity



Hetero-spin triplet component

$$(\uparrow\downarrow + \downarrow\uparrow)$$

Equal-spin triplet components

$$(\uparrow\uparrow - \downarrow\downarrow)$$

$$(\uparrow\uparrow + \downarrow\downarrow)$$

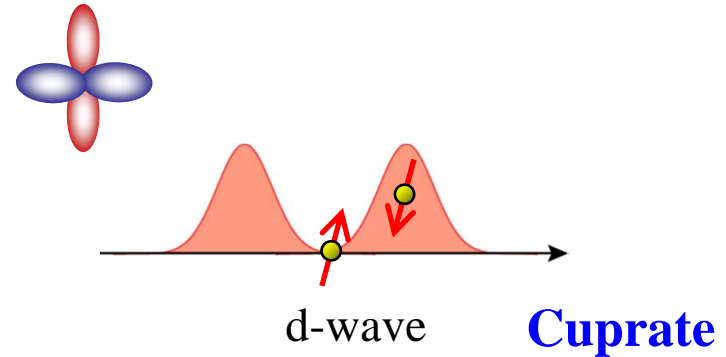
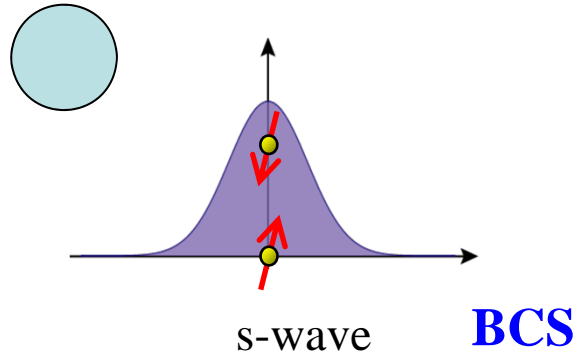
M. Eschrig, Physics Today (2011)

Conventional classification of the pairing symmetry

Spin-singlet Cooper pair



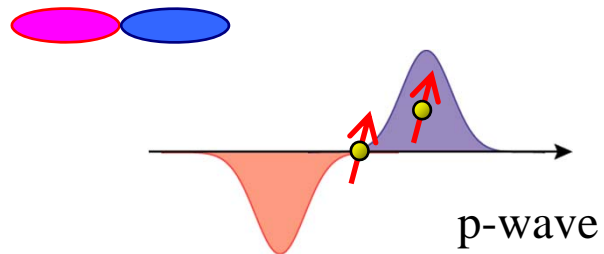
Even Parity



Spin-triplet Cooper pair



Odd Parity



In both cases, the pair amplitude is an even function of energy (or Matsubara frequency).

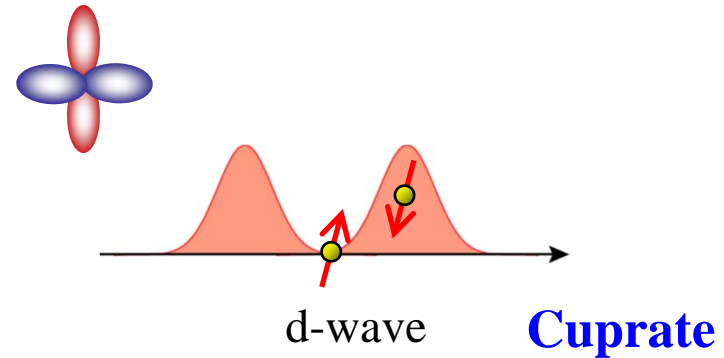
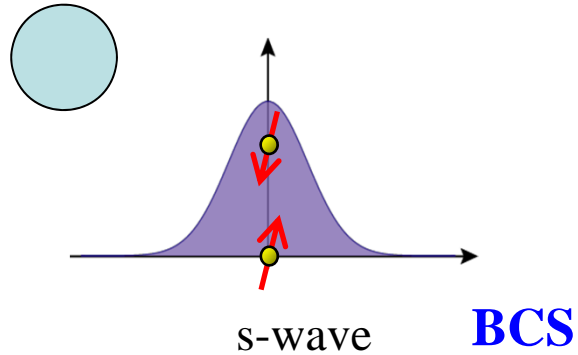


Conventional classification of the pairing symmetry

Spin-singlet Cooper pair



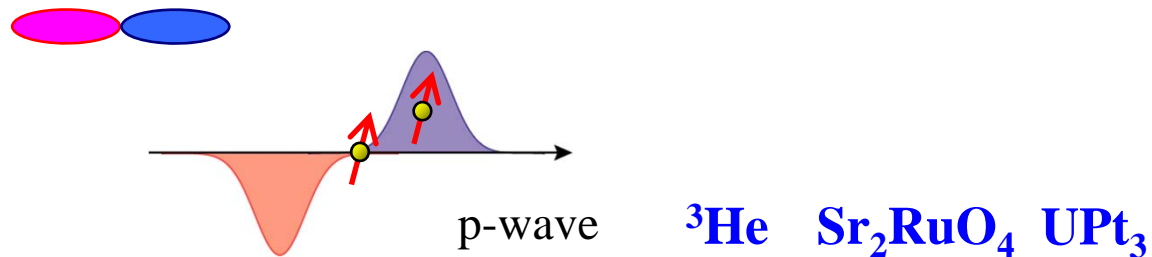
Even Parity



Spin-triplet Cooper pair



Odd Parity



However, the so-called **odd-frequency pairing states** when the pair amplitude is an odd function of energy can also exist.



Symmetry classification of induced pair potential

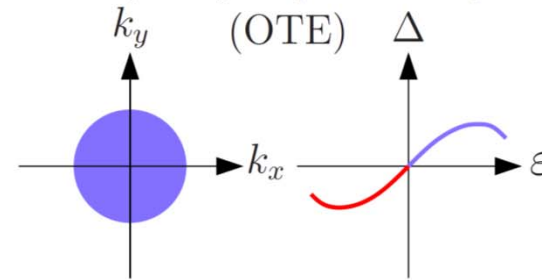
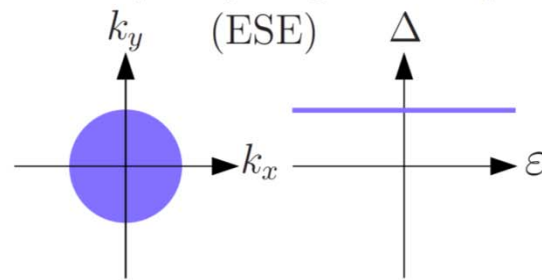
Fermi-Dirac statistics

Symmetry of pair wave functions:

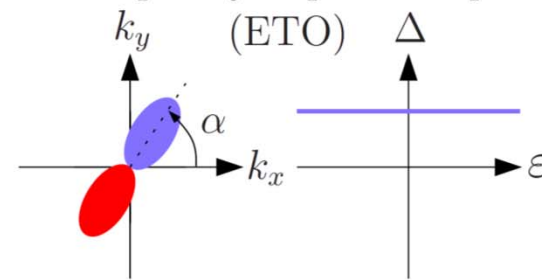
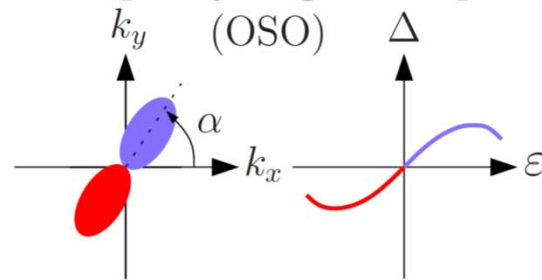
$$\mathbf{k} \otimes \sigma \otimes \omega = \text{odd}$$

	$F_{\sigma\sigma'}(\omega, k) = -F_{\sigma'\sigma}(-\omega, -k)$		
	$\omega \rightarrow -\omega$	$\sigma \leftrightarrow \sigma'$	$k \rightarrow -k$
<i>ESE</i>	+	-	+
<i>OSO</i>	-	-	-
<i>ETO</i>	+	+	-
<i>OTE</i>	-	+	+

Even frequency-singlet-even parity (ESE) Odd frequency-triplet-even parity (OTE)

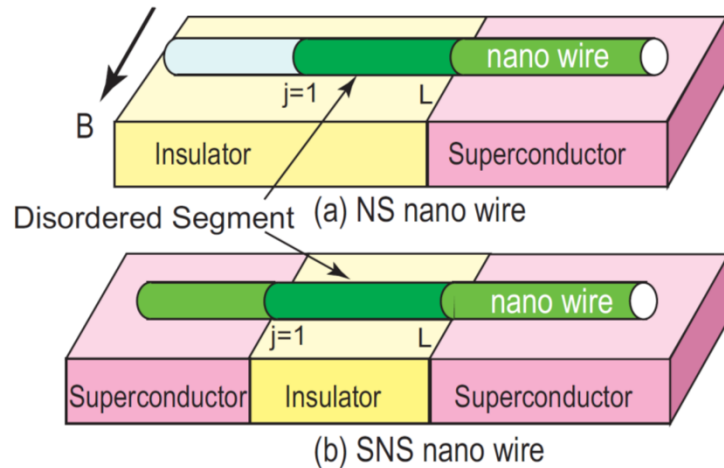


Odd frequency-singlet-odd parity (OSO) Even frequency-triplet-odd parity (ETO)

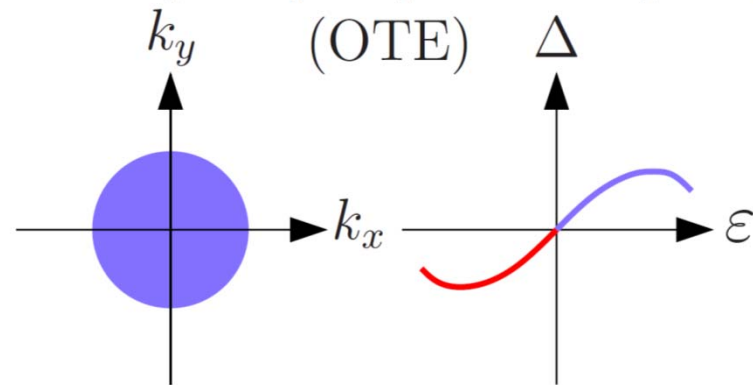


J. Linder et al., PRB (2008)

Odd-frequency pairing and Majorana state



Odd frequency-triplet-even parity



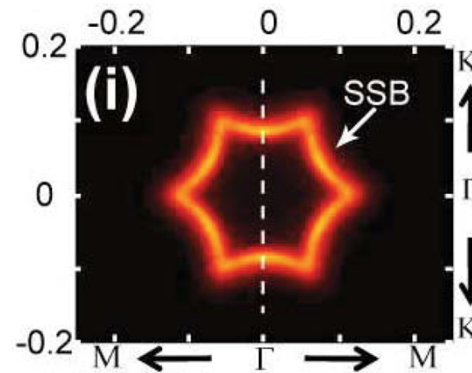
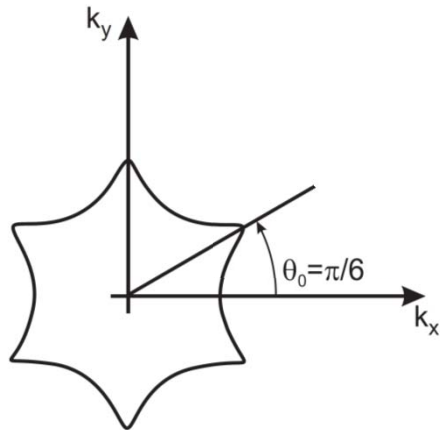
Asano, Tanaka, PRB (2013)

The physics behind the anomalous transport can be understood in terms of the odd-frequency Cooper pairing. We conclude that Majorana fermions and odd-frequency Cooper pairs in solids are two sides of a same coin.

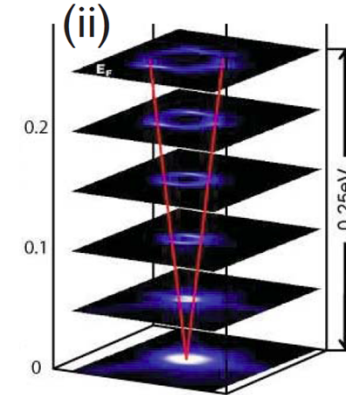
Hexagonal warping in 3D Topological insulators

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

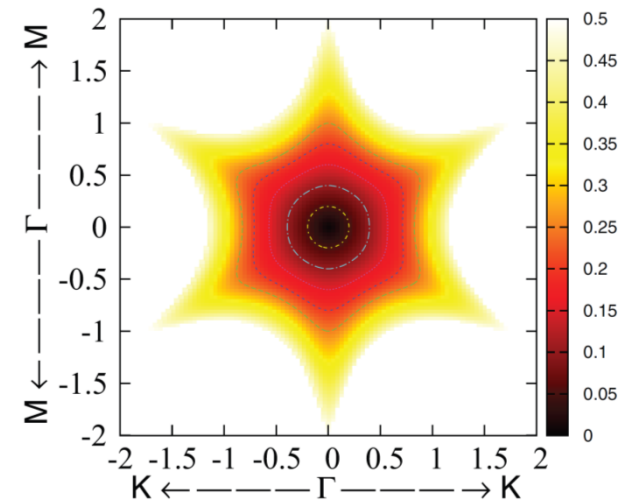
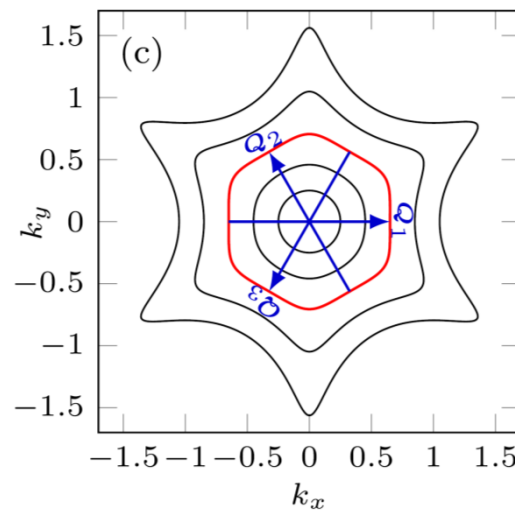
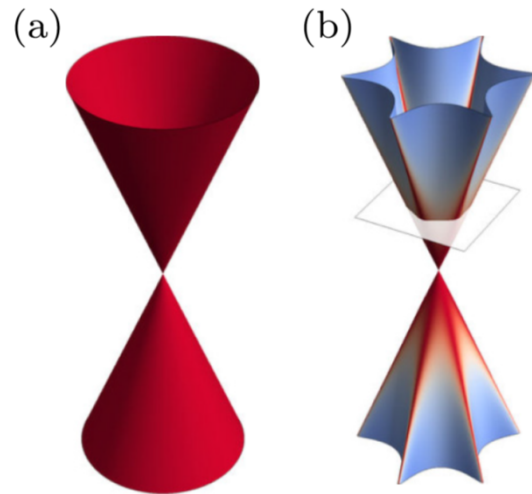
$$\hat{H}_w(\mathbf{k}) = \lambda k^3 \cos(3\theta) \hat{\sigma}_z$$



Fu, PRL (2009)



Chen et al., Science (2009)



Mendle, Kotetes, Schon, PRB (2015)

Li, Carbotte, PRB (2013)

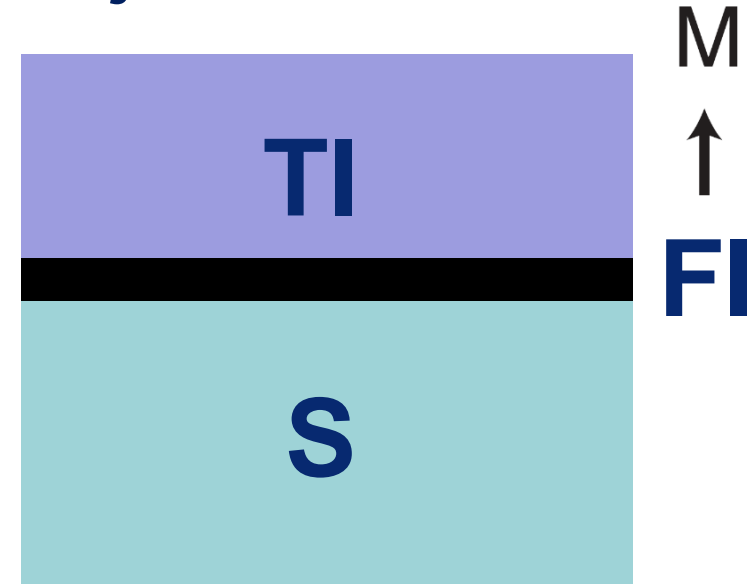
Model: S/ FI/ TI hybrid junction

Bogoliubov – de Gennes – Dirac Hamiltonian

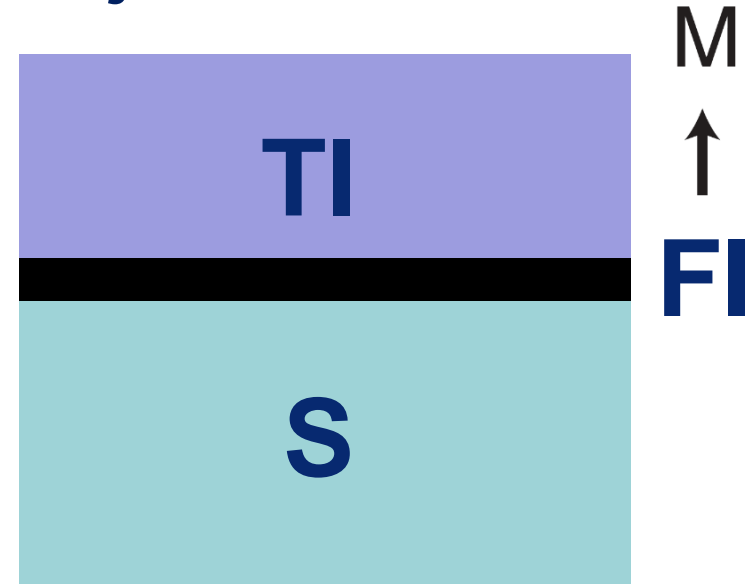
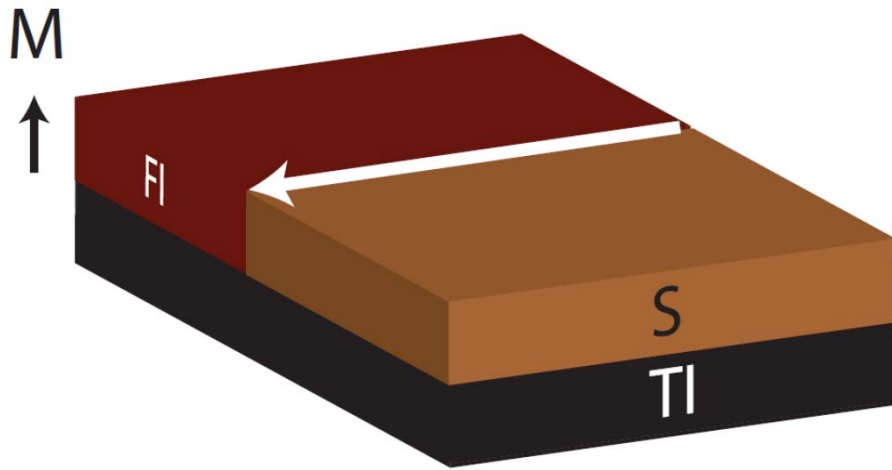
$$\check{H}_S(\mathbf{k}) = \begin{pmatrix} \hat{H}(\mathbf{k}) + M\hat{\sigma}_z & \hat{\Delta} \\ -\hat{\Delta} & -\hat{H}^*(-\mathbf{k}) - M\hat{\sigma}_z \end{pmatrix}$$

Green's function (Nambu + spin space)

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



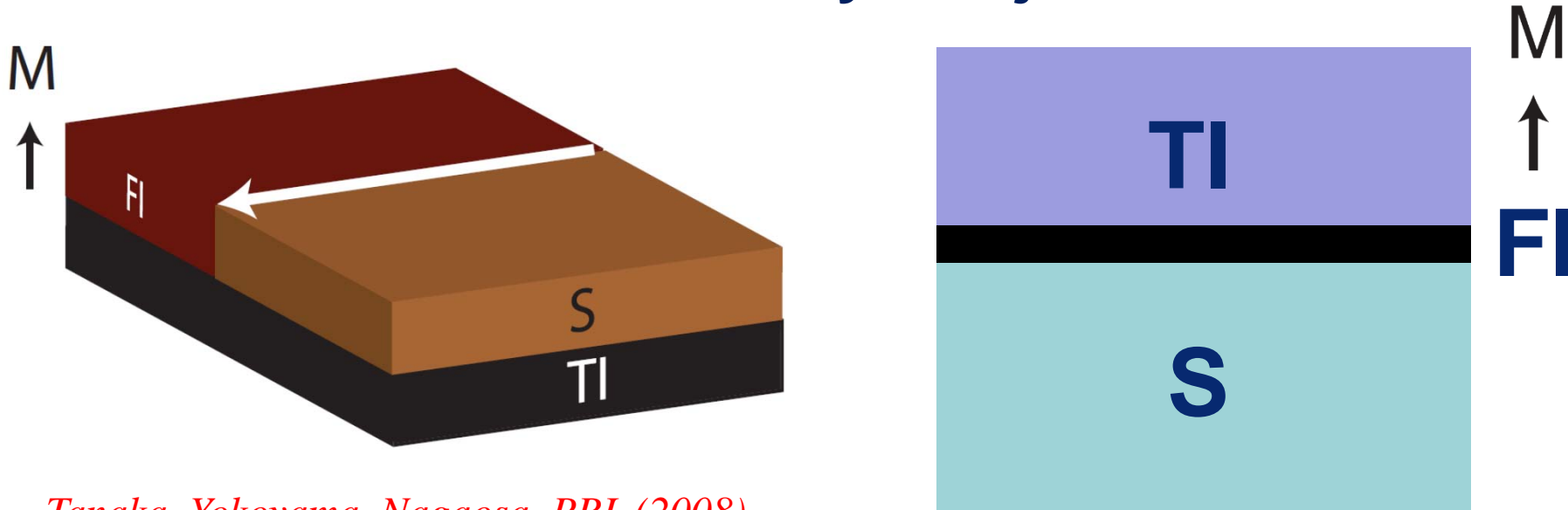
Model: S/ FI/ TI hybrid junction



Tanaka, Yokoyama, Nagaosa, PRL (2008)



Model: S/ FI/ TI hybrid junction



Tanaka, Yokoyama, Nagaosa, PRL (2008)

Anomalous Green's function

Bergeret, Volkov, Efetov, RMP (2005)

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

↓ ↓ ↓ ↓

$(\uparrow\downarrow - \downarrow\uparrow)$ singlet triplet triplet triplet $(\uparrow\downarrow + \downarrow\uparrow)$
 $(\uparrow\uparrow - \downarrow\downarrow)$ $(\uparrow\uparrow + \downarrow\downarrow)$



No warping

$$\check{H}_S(\mathbf{k}) = \begin{pmatrix} \hat{H}(\mathbf{k}) + M\hat{\sigma}_z & \hat{\Delta} \\ -\hat{\Delta} & -\hat{H}^*(-\mathbf{k}) - M\hat{\sigma}_z \end{pmatrix} \quad \hat{H}(\mathbf{k}) = -\mu + v(k_x\hat{\sigma}_y - k_y\hat{\sigma}_x)$$

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

Anomalous Green's function symmetry, Z is even in E and k

$$f_0 = \frac{\Delta}{Z} (E^2 + M^2 - \mu^2 - \Delta^2 - v^2k^2), \quad (\uparrow\downarrow - \downarrow\uparrow) \quad \mathbf{ESE}$$

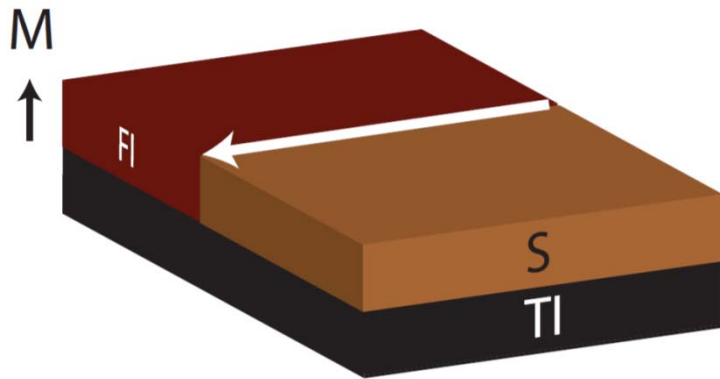
$$f_x = \frac{2\Delta}{Z} kv [\mu \sin(\theta) + iM \cos(\theta)], \quad (\uparrow\uparrow - \downarrow\downarrow) \quad \mathbf{ETO}$$

$$f_y = -\frac{2\Delta}{Z} kv [\mu \cos(\theta) - iM \sin(\theta)], \quad (\uparrow\uparrow + \downarrow\downarrow) \quad \mathbf{ETO}$$

$$f_z = \frac{2\Delta}{Z} EM. \quad (\uparrow\downarrow + \downarrow\uparrow) \quad \mathbf{OTE} \quad \mathbf{Majorana mode}$$

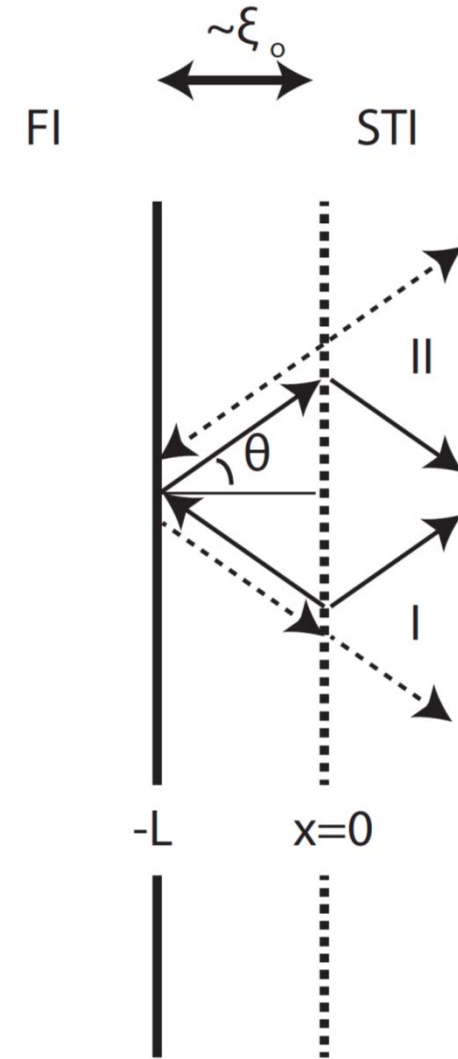
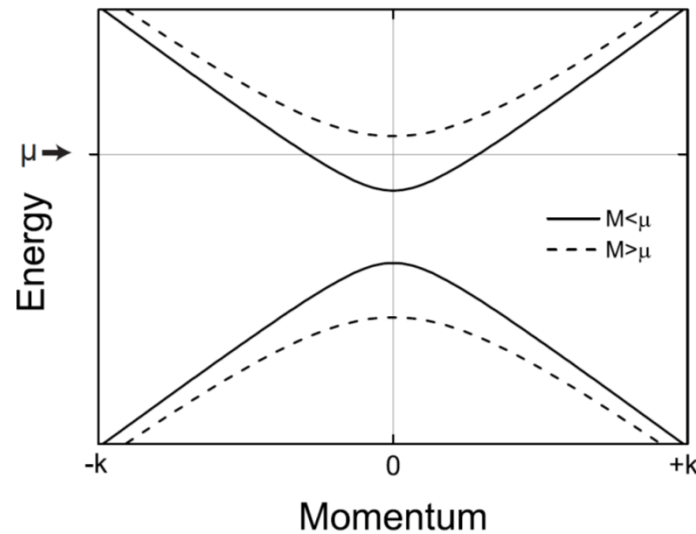
Vasenko, Golubov, Silkin, Chulkov, JETP Lett. (2017)

Majorana fermion realization



$$\frac{E}{\Delta} = -\sin(\theta)$$

$$= -k_y/|k|.$$



Snelder, Golubov, Asano, Brinkman, J. Phys.: Cond. Mat. (2015)

Finite warping

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

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

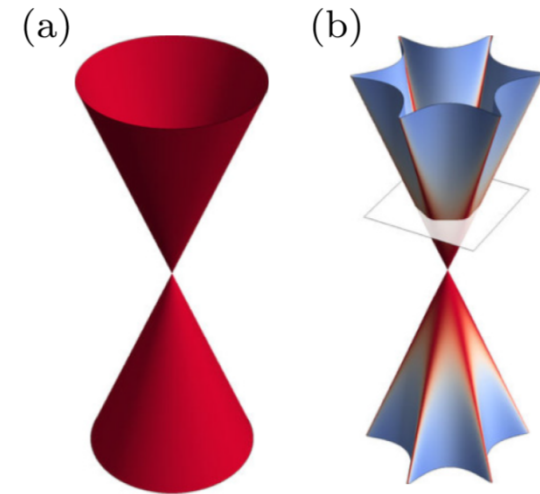
$$\hat{G}_{\text{eh}} = i(f_0\hat{\sigma}_0 + f_x\hat{\sigma}_x + f_y\hat{\sigma}_y + f_z\hat{\sigma}_z)\hat{t}_y$$

$$f_i = f_i^+ + f_i^-$$

Spin-singlet component $(\uparrow\downarrow - \downarrow\uparrow)$

$$f_0^+ = \left(E^2 + M^2 - \mu^2 - \Delta^2 - E_S^2 \right) F_{\text{even}}/2, \quad \mathbf{ESE}$$

$$f_0^- = \left(E^2 + M^2 - \mu^2 - \Delta^2 - E_S^2 \right) F_{\text{odd}}/2. \quad \mathbf{OSO}$$



Finite warping

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

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

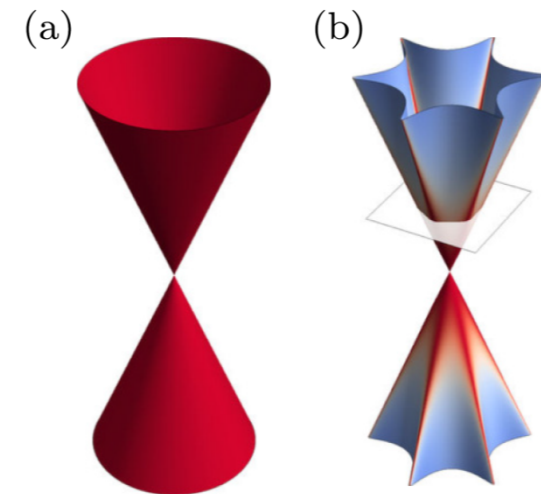
Equal spin triplet components $(\uparrow\uparrow - \downarrow\downarrow)$ $(\uparrow\uparrow + \downarrow\downarrow)$

$$f_x^+ = kv[\mu \sin(\theta) + iM \cos(\theta)] F_{\text{even}}, \quad \mathbf{ETO}$$

$$f_x^- = kv[\mu \sin(\theta) + iM \cos(\theta)] F_{\text{odd}}, \quad \mathbf{OTE}$$

$$f_y^+ = -kv[\mu \cos(\theta) - iM \sin(\theta)] F_{\text{even}}, \quad \mathbf{ETO}$$

$$f_y^- = -kv[\mu \cos(\theta) - iM \sin(\theta)] F_{\text{odd}}, \quad \mathbf{OTE}$$



Finite warping

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

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

Hetero-spin triplet component

$$(\uparrow\downarrow + \downarrow\uparrow)$$

$$f_z = f_z^- + f_z^+,$$

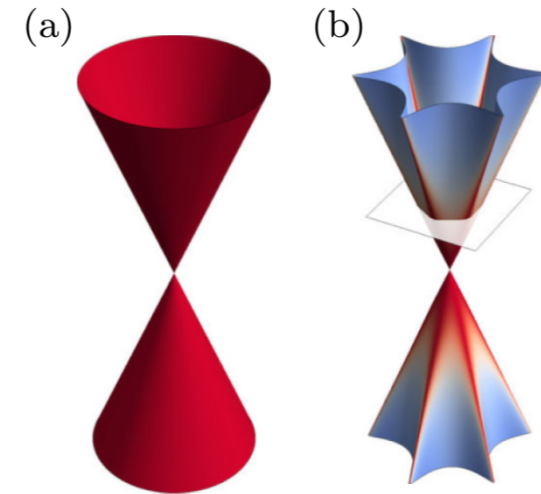
$$f_z^- = EMF_{\text{even}} - \mu\lambda k^3 \cos(3\theta)F_{\text{odd}},$$

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

OTE

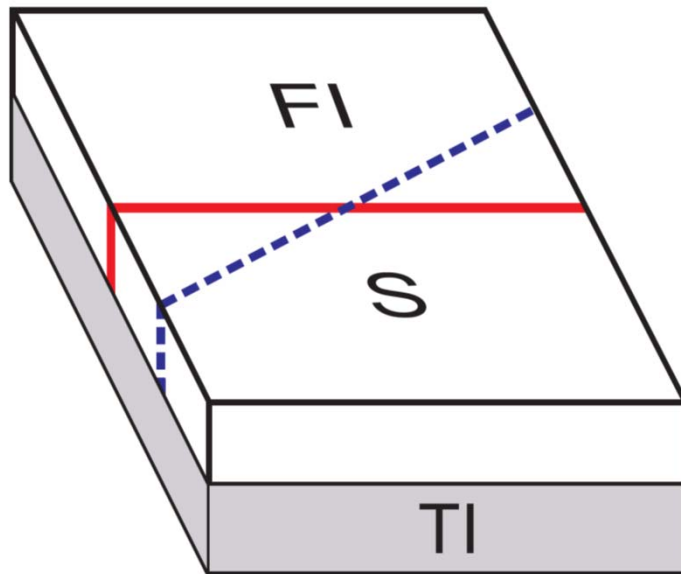
ETO

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

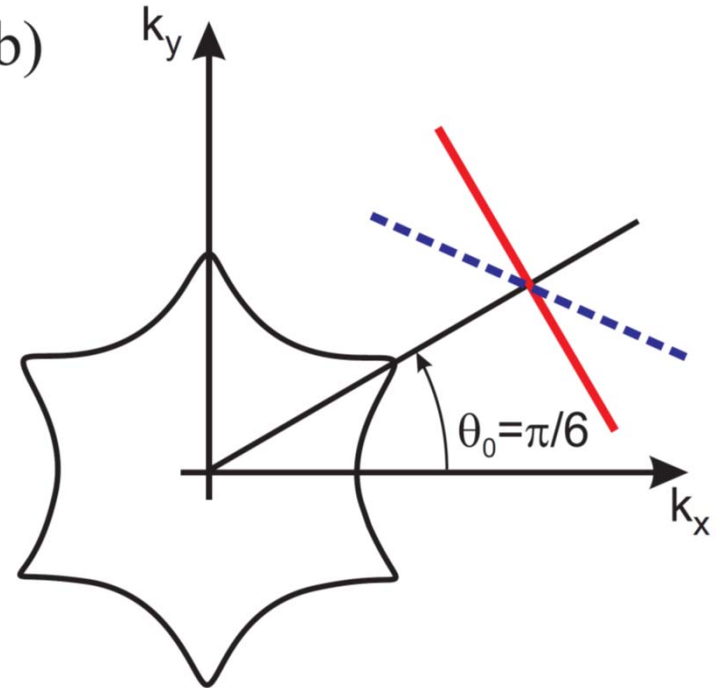


Majorana fermion (?) and warping

a)



b)

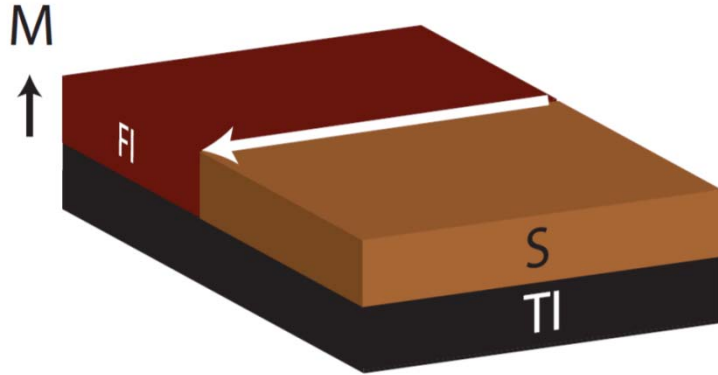


Vasenko, Golubov, Silkin, Chulkov, J. Phys.: Cond. Matt. (2017)

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

Spontaneous supercurrent

$$\hat{H}_M(\mathbf{k}) = -\mu + v(k_x \hat{\sigma}_y - k_y \hat{\sigma}_x) + \lambda k^3 \cos(3\theta) \hat{\sigma}_z + M \hat{\sigma}_z$$



Let us project this Hamiltonian on the S/FI interface, i.e., on the y axis. Then the effective one-dimensional Hamiltonian for electronic states at the S/FI interface will look like ($k_x \sim 0$),

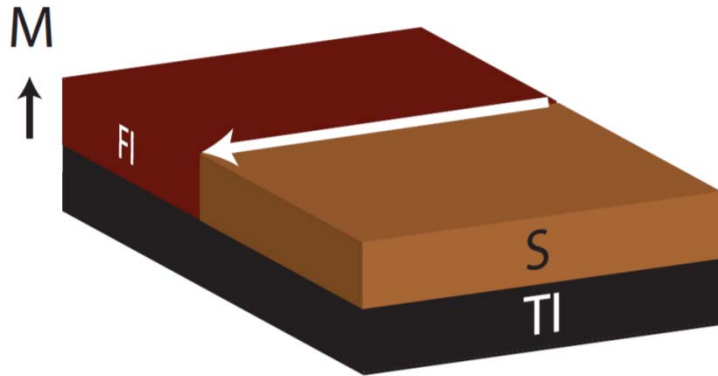
$$\hat{H}_{\text{eff}}(k_y) = -\mu - vk_y \hat{\sigma}_x + \hat{\sigma}_z \lambda k_y^3 \cos(3\theta) + \hat{\sigma}_z M$$

From the viewpoint of the time reversal and spatial symmetries, it is equivalent to the following one dimensional Hamiltonian of a topological nanowire,

$$\hat{H}(\mathbf{k}) = -\mu + vk_x \hat{\sigma}_y + \hat{\sigma}_x M_x + \hat{\sigma}_y M_y + \hat{\sigma}_z M_z$$

Spontaneous supercurrent

$$\hat{H}_M(\mathbf{k}) = -\mu + v(k_x \hat{\sigma}_y - k_y \hat{\sigma}_x) + \lambda k^3 \cos(3\theta) \hat{\sigma}_z + M \hat{\sigma}_z$$



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From the viewpoint of the time reversal and spatial symmetries, it is equivalent to the following one dimensional Hamiltonian of a topological nanowire,

$$\hat{H}(\mathbf{k}) = -\mu + vk_x \hat{\sigma}_y + \hat{\sigma}_x M_x + \hat{\sigma}_y M_y + \hat{\sigma}_z M_z$$

Spontaneous supercurrent at zero phase difference.

Nesterov, Houzet, Meyer, PRB (2016)

Review

- We discuss singlet to triplet mixing in proximized 3D topological insulators with warped surface state
- We speculate on the selection rule for Majorana Fermion realization in S/FI structures formed on the surface of the TI: S/FI boundary should be properly aligned with respect to the snowflake contour.
- Spontaneous currents in S/TI hybrids at nonzero warping.

Thank you!

