The main idea is to convey to the audience the feeling
that trying to understand the basic mathematics of Physics
can be a way towards the understanding of a basic unity of the laws of Nature.

Beppe Morandi

From Integer Quantum Hall effect to Majorana Fermions in Topological Materials.

Bologna, 24-25 novembre 2017

A. Tagliacozzo (Universita' di Napoli "Federico II")

P.Lucignano, *G.Campagnano, F.Trani, D.Giuliano (Cz), A.Mezzacapo (now IBM Yorktown),*
exp. groups of F.Tafuri (Napoli) & F.Lombardi(Chalmers)

Michela di Stasio,

SISSA phd diploma 1993:

From quantum Spins to correlated fermions: a new strong coupling method

Il ricordo del mio austero, rigoroso,
a volte iroso, sensibile, attento,
sempre generoso correlatore di tesi resta immutato nel mio cuore.
Ho imparato tantissimo da Beppe professionalmente ma il privilegio di averlo frequentato, anche se per un breve periodo, da studente fuori sede e quindi anche al di là delle mura universitarie è stato e resta tuttora un'esperienza preziosa. Mi dispiace di non essere con voi ma vi abbraccio tutti con affetto.

Content: **from two bands, Time Reversal Invariant (TRI) Topological Insulators to Majorana excitations**

- *1-2-D models for Topological systems:*
- p-wave pairing in spinless systems allows for Majorana real fermion, zero energy excitations
- *3D TRI Topological Insulators*
- helicity of topological states at the boundaries
- d-wave superconductive proximity of a wire
- Majorana bound state at a vortex core
- Fermi arcs in Weyl semimetals

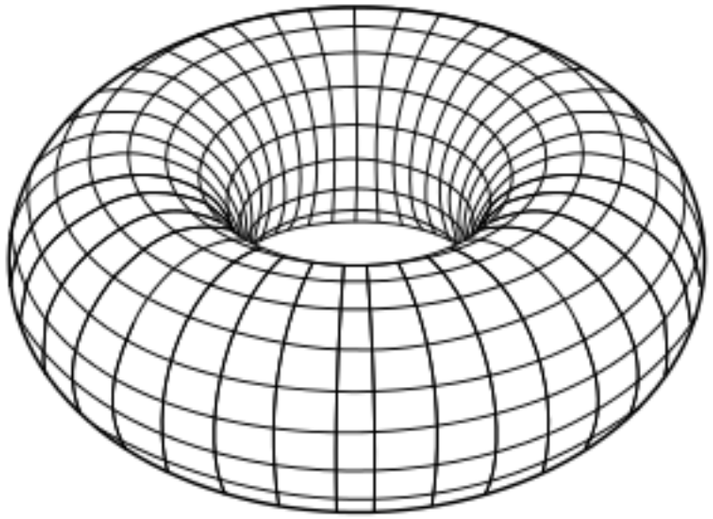
The correspondence bulk-edges has been taken over in the Quantum Spin Hall 2D-systems, in the 3D-Topological Insulators which have Dirac states in the bulk gap, crossing the Fermi energy, localized at the boundaries and in Weyl semimetal.

Integer Hall conductance as the integral of the Berry curvature over the BZ

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\int\int_{BZ} dk_x\, dk_y\, \mathcal{F}_{xy}(k) = \frac{e^2}{h}\mathcal{C}_1$$

$$\mathcal{F}_{xy}(k) = \frac{\partial A_y(k)}{\partial k_x} - \frac{\partial A_x(k)}{\partial k_y}$$

$$A_i = -i \sum_{a \in\, filled\, bands} \left\langle a\,\vec{k} \left| \frac{\partial}{\partial k_i} \right| a\,\vec{k} \right\rangle$$



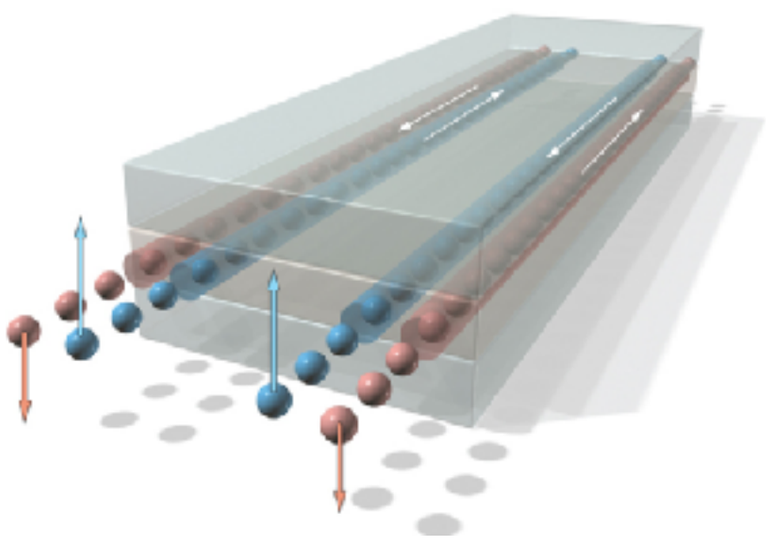
BZ

A non zero Chern number as an obstruction to Stokes' Theorem over the whole BZ

for Time reversal invariant systems $\mathcal{F}\left(-\vec{k}\right) = -\mathcal{F}\left(\vec{k}\right)$ $\Rightarrow$ $\mathcal{C} = 0$

non trivial Z_2 index must be an obstruction to defining the TR-smooth gauge between Kramers degenerate states

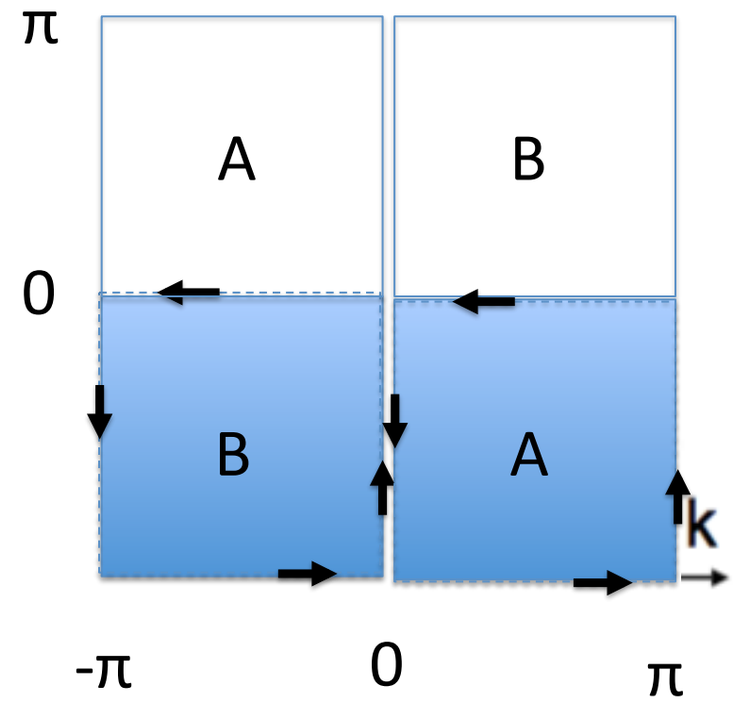
QSH : HgTe quantum well



in half the BZ

$$\left|u_a^I(-\vec{k})\right\rangle = \Theta\left|u_a^{II}(\vec{k})\right\rangle$$

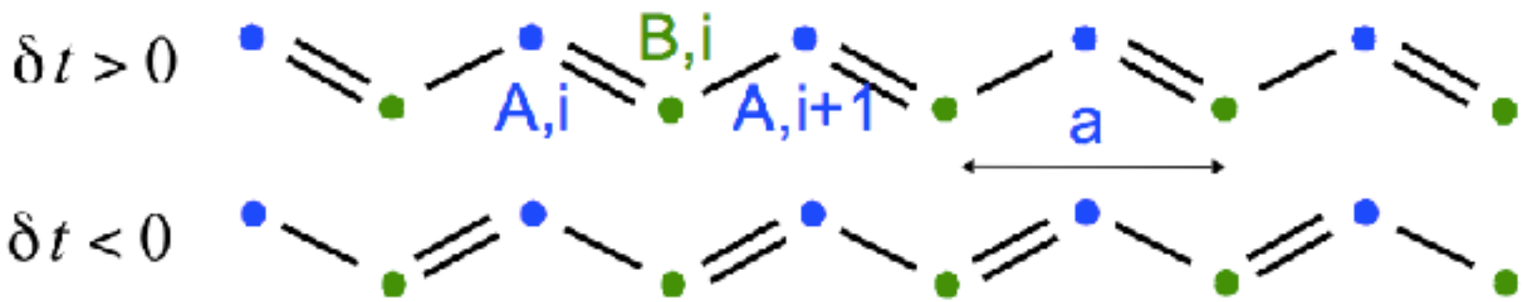
$$\left|u_a^{II}(-\vec{k})\right\rangle = -\Theta\left|u_a^{I}(\vec{k})\right\rangle$$

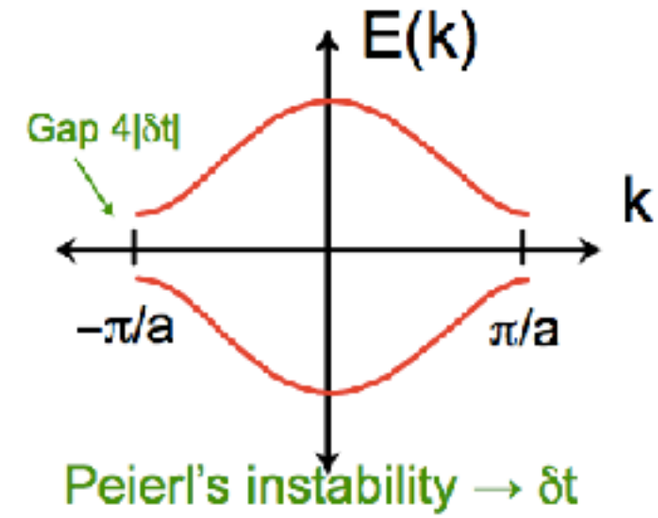


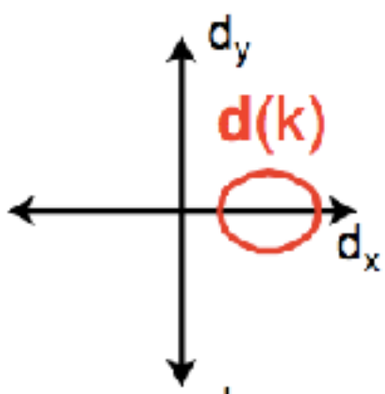
$\neq$

Bulk-edge correspondence: topologically protected edge states

$$H = \sum_i (t+\delta t)c^{\dagger}_{Ai}c_{Bi} + (t-\delta t)c^{\dagger}_{Ai+1}c_{Bi} + h.c.$$

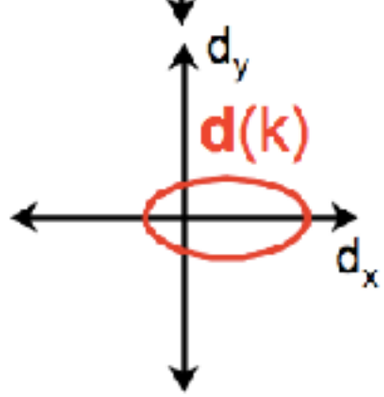






δt>0 : Berry phase 0

P = 0



δt<0 : Berry phase π

P = e/2

$$H = \sum_k \mathbf{H}(k) \;\; with \;\; \mathbf{H}(k) = \vec{d}(k)\cdot\vec{\tau}$$

$$d_x = t_+ + t_- \cos k, \qquad d_y = t_- \sin k, \qquad d_z = 0$$

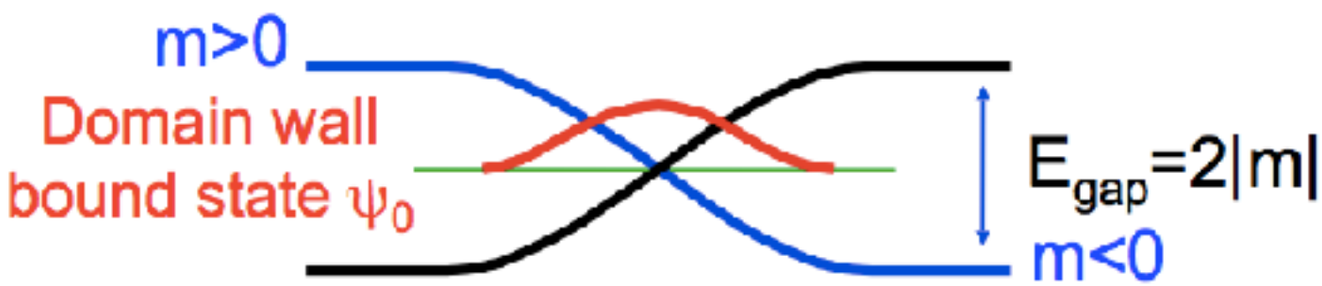
$$\vec{g} = \frac{\vec{d}}{|\vec{d}\,|}$$

$$\mathcal{C}_1 = \frac{1}{4\pi}\int_{\mathcal{S}^2} d\theta d\varphi\, \vec{g}(\hat{n})\cdot[\,\partial_\theta \vec{g}(\hat{n}) \times \partial_\varphi \vec{g}(\hat{n})\,] = \int_{\mathcal{S}^2} d\Omega/4\pi.$$

zero energy real fermion at the boundary in the SSH model

Zero mode : topologically protected eigenstate at E=0

(Jackiw and Rebbi 76, Su Schrieffer, Heeger 79)

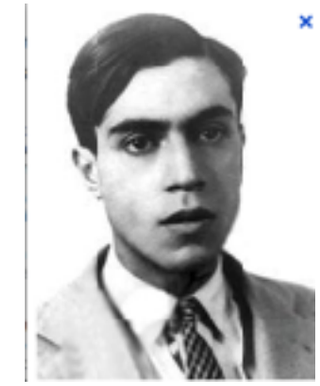


$$\psi_0(x) = e^{-\int_0^x m(x')dx'/v_F} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$H\psi_0(x) = [-iv_F\sigma_y\partial_x + m(x)\sigma_x]\ \psi_0(x) = 0$$

$$m(x)\,(i\,\sigma_y + \sigma_x)\,\phi_0 = 0: \quad \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}\phi_0 = 0, \quad \rightarrow \phi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

neutral fermion requires superconductivity



Note that in BCS:

$$\gamma_{k0} = u_k \, c_{k\uparrow} - v_k \, c^\dagger_{-k\downarrow}$$

$$\gamma_{k1} = u_k \, c_{-k\downarrow} + v_k \, c^\dagger_{k\uparrow}$$

Time Reversal implies that:

$$u^*_{-k} = v_k, \quad v^*_{-k} = -u_k$$

so that

spin reverses between $\gamma^\dagger_{\vec{k}0}, \ \gamma_{-\vec{k}0}$ **!**

$$\gamma_{\vec{k}} = u_{\vec{k}} c_{\vec{k}} - v_{\vec{k}} c_{-\vec{k}}{}^\dagger$$

$$\gamma_{\vec{k}}{}^\dagger = u^*_{\vec{k}} c_{\vec{k}}{}^\dagger - v^*_{\vec{k}} c_{-\vec{k}}$$

model has to be spinless !

provided: $u^*_{-\vec{k}} = -v_{\vec{k}}, \quad v^*_{-\vec{k}} = -u_{\vec{k}}$

is: $$\gamma^\dagger_{\vec{k}} = \gamma_{-\vec{k}}$$

spinless requires p-wave pairing !

spinful singlet (s-wave) pairing

$$\Delta \left(c^\dagger_{-k\downarrow} c^\dagger_{k\uparrow} - c^\dagger_{-k\uparrow} c^\dagger_{k\downarrow} \right)$$

$$k \uparrow \rightarrow -k \downarrow \quad \Rightarrow \quad \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - c^\dagger_{k\downarrow} c^\dagger_{-k\uparrow} \right)$$

spinless (p-wave) pairing

$$\Delta[k] \left(c^\dagger_{k} c^\dagger_{-k} + c^\dagger_{-k} c^\dagger_{k} \right)$$

k ⟶ -k ⇒ Δ[-k] = -Δ[k]

Bogolubov-de Gennes Hamiltonian

with $\hat{\Delta}^T = -\hat{\Delta}$

$$H_{MF} = \begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^T \end{pmatrix}$$

$$\sigma_x H_{MF} \sigma_x = \begin{pmatrix} -h^T & \Delta^\dagger \\ \Delta & h \end{pmatrix} \equiv -H^*_{MF}$$

$$\mathcal{H}_k = \hat{h}(k) \cdot \vec{\sigma} \qquad h_{x,y}(-k) = -h_{x,y}(k), \qquad h_z(-k) = h_z(k)$$

$$H = -\mu \sum_x c_x^\dagger c_x - \frac{1}{2} \sum_x \left[t\, c_x^\dagger c_{x+1} + \Delta\, e^{i\phi} c_x c_{x+1} + H.c. \right]$$

Kitaev model ('97)

$$\mathcal{H}_k = \hat{h}(k) \cdot \vec{\sigma}$$

$$\hat{h}(0) = s_0 \hat{z}, \qquad \hat{h}(\pi) = s_\pi \hat{z}$$

Z_2 **topological invariance**

$$\nu = s_0\, s_\pi$$

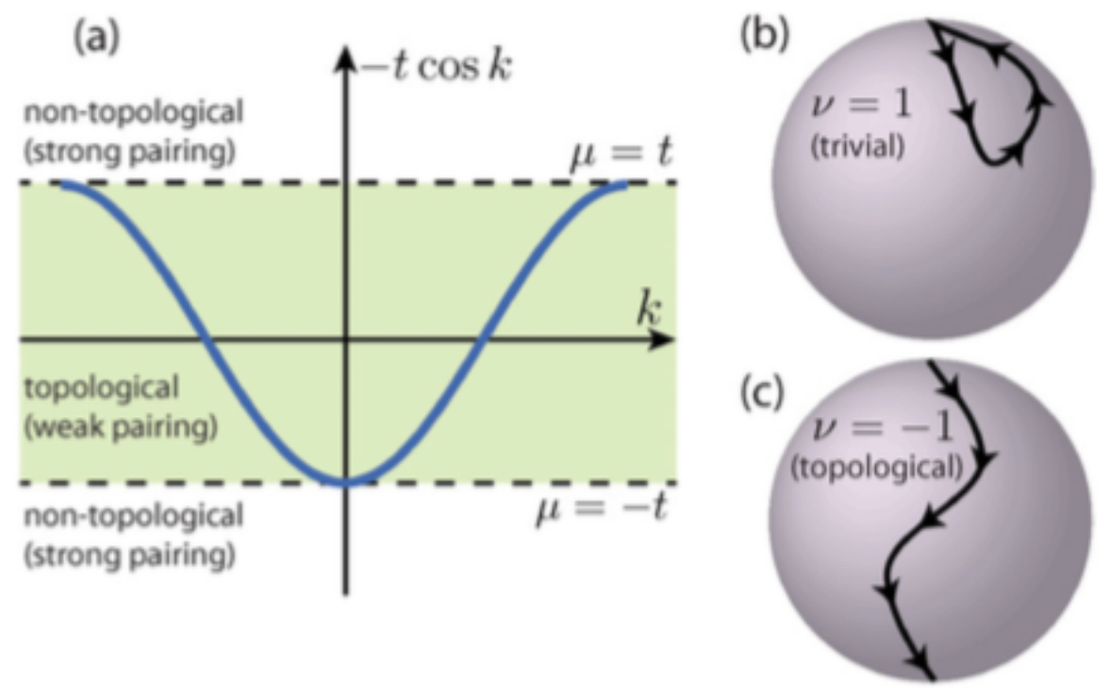


Figure 1. (*a*) Kinetic energy in Kitaev's model for a 1D spinless p-wave superconductor. The p-wave pairing opens a bulk gap except at the chemical potential values $\mu = \pm t$ displayed above. For $|\mu| > t$ the system forms a non-topological strong pairing phase, while for $|\mu| < t$ a topological weak-pairing phase emerges. The topological invariant ν distinguishing these states can be visualized by considering the trajectory that $\hat{h}(k)$ (derived from equation (10)) sweeps on the unit sphere as k varies from 0 to π; (*b*) and (*c*) illustrate the two types of allowed trajectories.

J. Alicea, Rev. Mod. Phys. 2012
A. Kitaev, Annals of Physics 2003

Bogolubov-de Gennes Hamiltonian

with $\hat{\Delta}^T = -\hat{\Delta}$

$$H_{MF} = \begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^T \end{pmatrix}$$

$$\sigma_x \, H_{MF} \sigma_x = \begin{pmatrix} -h^T & \Delta^\dagger \\ \Delta & h \end{pmatrix} \equiv -H^*_{MF}$$

$$H_{MF}\psi_n = \epsilon_n \psi_n, \quad H_{MF}\sigma_x \psi_n^* = \sigma_x^2 H_{MF} \sigma_x \psi_n^* = -\sigma_x H^*_{MF} \psi_n^* = -\epsilon_n \sigma_x \psi_n^*$$

$$\psi_n = \begin{pmatrix} u_n \\ v_n \end{pmatrix} \;\rightarrow\; \sigma_x \psi_n^* = \begin{pmatrix} v_n^* \\ u_n^* \end{pmatrix}$$

$$\sigma_x \psi^{0*} = \psi^0 \quad \rightarrow \quad \psi^0 = \begin{pmatrix} u_0 + v_0^* \\ v_0 + u_0^* \end{pmatrix} \equiv \begin{pmatrix} w_0 \\ {w_0}^* \end{pmatrix}$$

$$\gamma_0^\dagger = w_0 \, a_0^\dagger + w_0^* \, a_0 \equiv \gamma_0$$

Majoranas come always in pairs and give two degenerate ground states of opposite parity

- bound state of two Majorana in a π-Josephson Junction (1D)

- bound Andreev state in 2D when proximity is p-ip

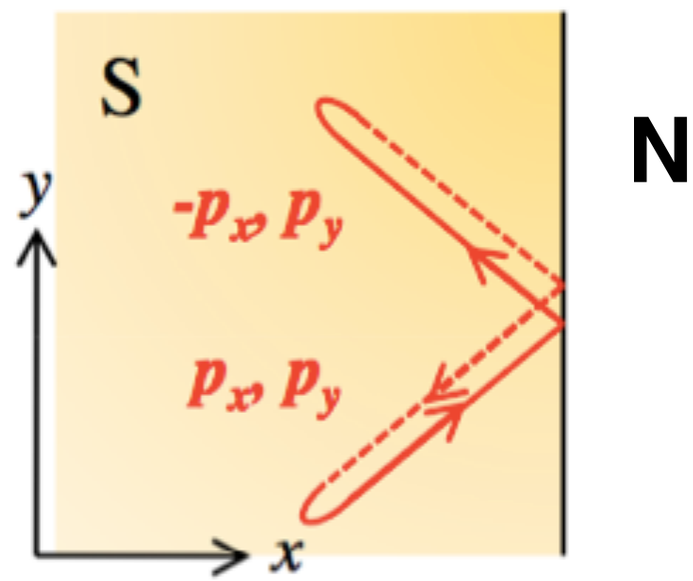
$$\Delta(\vec{p}) = \Delta_0 (p_x - i p_y) \equiv \Delta_0 \cdot p \cdot e^{i\phi(\vec{p})}$$

$$r_{he}(\epsilon, \vec{p}) = \alpha\, e^{-i\phi(\vec{p})}$$

$$r_{eh}(\epsilon, \vec{p}) = \alpha\, e^{i\phi(\vec{p})}$$

$$\alpha = e^{-i \arccos(\epsilon/|\Delta(\vec{p})|)}\, e^{-i\chi/2}$$

$$\phi(\vec{p}) = -\arctan p_y/p_x$$



Bohr-Sommerfeld quantization:

$$1 = r_{eh}(\epsilon, p_x, p_y)\; r_{he}(\epsilon, -p_x, p_y)$$

$$= e^{-2i \arccos(\epsilon/\Delta(\vec{p})) - i\phi(-p_x, p_y) + i\phi(p_x, p_y)}\; e^{-i\chi}$$

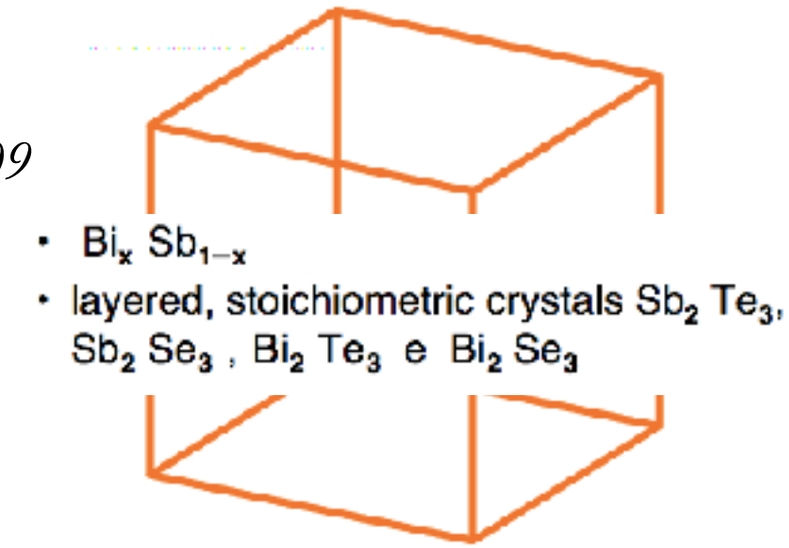
admits solution with $\epsilon = \Delta_0\, p_y$ provided the phase acquired in the loop is $\chi = \pi$.
This is indeed the case at surfaces of Topological Insulators

Two bands model Hamiltonian for TI

Zhang et al. 2009

minimal model in the continuum limit:

$$\mathcal{H}_0[\vec{r}] = \hbar v_F \begin{pmatrix} -\mathcal{M}-\mu & i\partial_z & 0 & i(\partial_x - i\partial_y) \\ i\partial_z & \mathcal{M}-\mu & i(\partial_x - i\partial_y) & 0 \\ 0 & i(\partial_x + i\partial_y) & -\mathcal{M}-\mu & -i\partial_z \\ i(\partial_x + i\partial_y) & 0 & -i\partial_z & \mathcal{M}-\mu \end{pmatrix}$$



$$(\psi_{g\uparrow}\,,\psi_{u\uparrow}\,,\psi_{g\downarrow}\,,\psi_{u\downarrow}\,)$$

Bulk bands dispersion $\quad E = \pm\sqrt{M^2 + k^2 + k_z^2}$ at the $\bar{\Gamma}$ point

$$\Theta\mathcal{H}_0(\vec{k})\Theta^{-1} = \mathcal{H}_0(-\vec{k})$$ TR invariant

$$\Xi\mathcal{H}_0(\vec{k})\Xi^{-1} = -\mathcal{H}_0(\vec{k})$$ p-h symmetric (μ=0)

$$\Gamma\mathcal{H}_0(\vec{k})\Gamma^{-1} = -\mathcal{H}_0(-\vec{k})$$ transforms p-h (μ=0) conserving helicity

$\Gamma = i\,\Theta\Xi$ *is the chirality*

$$\Theta = \mathcal{I} \otimes i\tau_y\mathcal{K}, \quad \Xi = -i\sigma_y \otimes \tau_x\mathcal{K}, \quad \Gamma = \sigma_y \otimes \tau_z$$

states localised at surfaces appear in the insulating gap

Projecting H onto the L,R chiral space:

$$\Pi_L = \frac{(\mathbf{1}-\Gamma)}{2} \qquad \Pi_R = \frac{(\mathbf{1}+\Gamma)}{2}$$

$$\mathcal{H}_0[M]\,\Pi_L = \begin{pmatrix} 0 & (\sigma_x - i\,\sigma_z)\,k_- \\ (\sigma_x + i\,\sigma_z)\,k_+ & 0 \end{pmatrix} \qquad k_\pm = k_x \pm i\,k_y$$

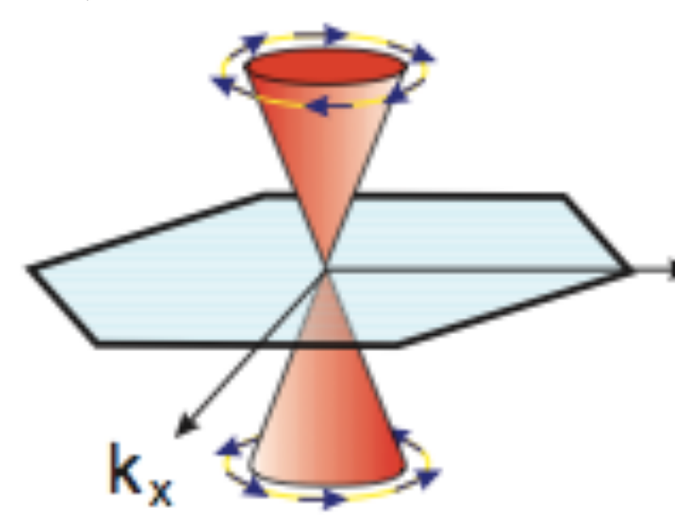
$$\mathcal{H}_0[-M]\,\Pi_R = \begin{pmatrix} 0 & (\sigma_x + i\,\sigma_z)\,k_- \\ (\sigma_x - i\,\sigma_z)\,k_+ & 0 \end{pmatrix}$$

$$E = \pm k$$

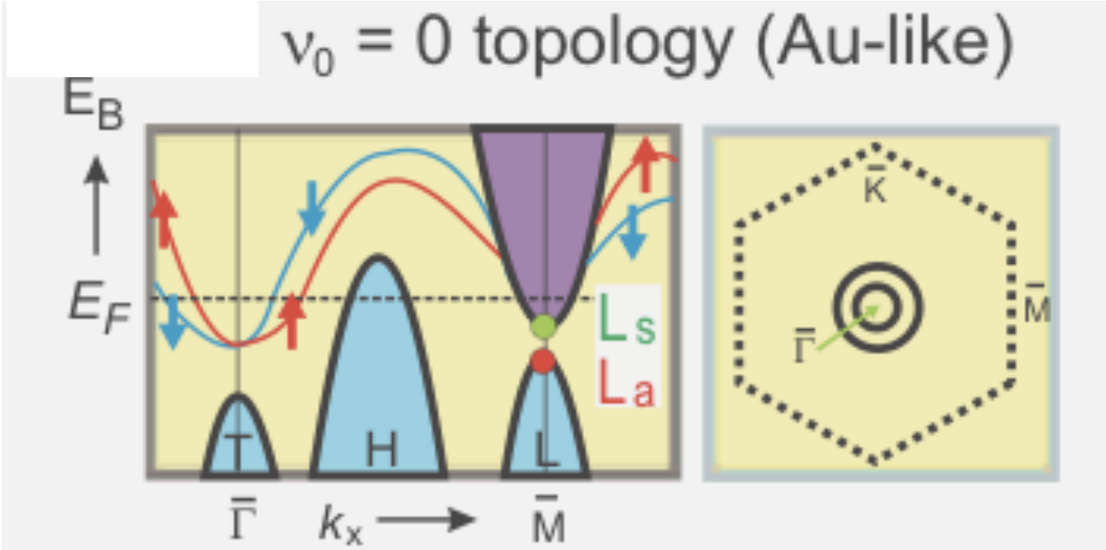
chirality fixes an internal structure: $(\psi_{g\uparrow}\,,\psi_{u\uparrow}\,,\psi_{g\downarrow}\,,\psi_{u\downarrow}\,)$

L-chiral $\quad \psi_{g\uparrow} - i\,\psi_{u\uparrow}, \quad \psi_{u\downarrow} + i\,\psi_{g\downarrow}$

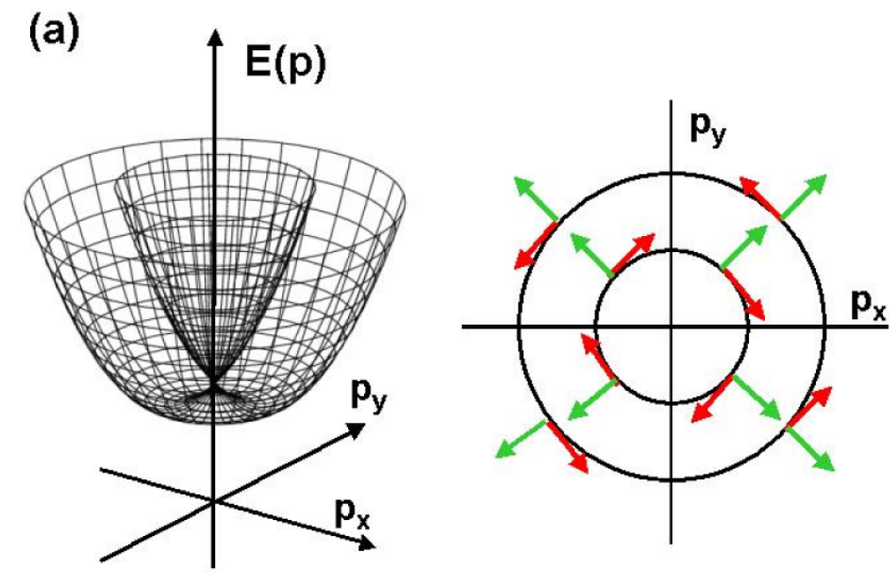
R-chiral $\quad \psi_{g\uparrow} + i\,\psi_{u\uparrow}, \quad \psi_{u\downarrow} - i\,\psi_{g\downarrow}$



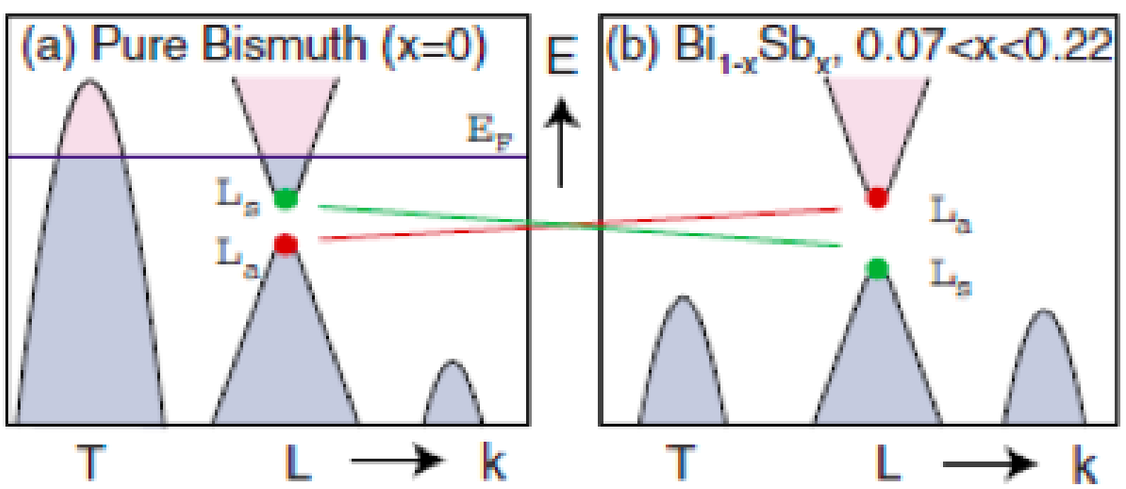
$$H[M;z=0]\Pi_L = -H[-M;z=0]\Pi_R = \begin{pmatrix} 0 & k_- \\ k_+ & 0 \end{pmatrix} = \vec{\sigma}\cdot\vec{k}$$



Rashba SO in 2DEG



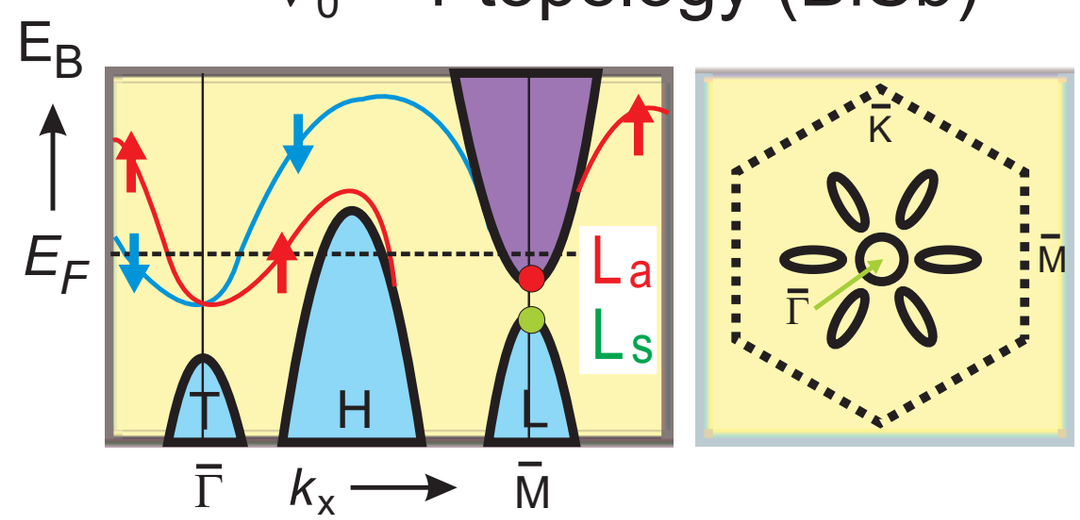
from metal to semiconductor



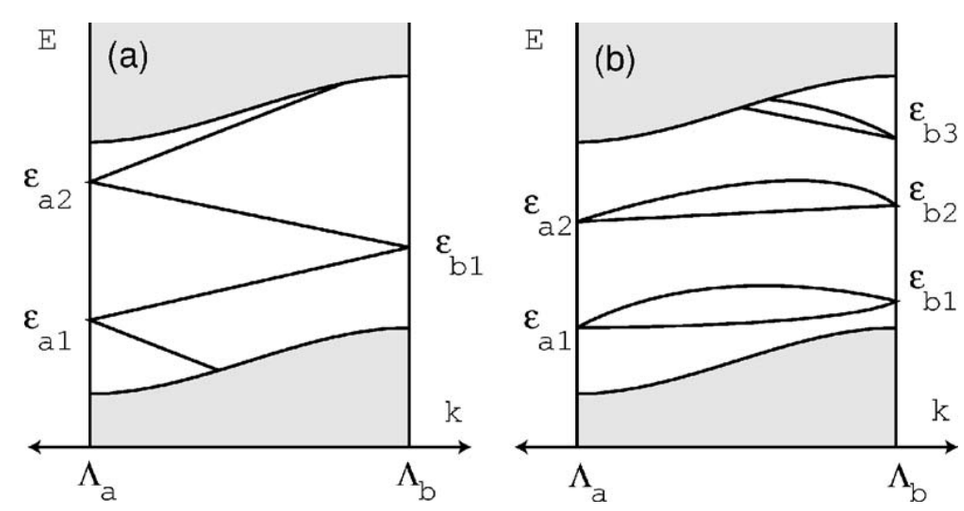
bulk bands invers with Sb

At interfaces (3-d), edges (2-d), the Fermi energy can intersect an odd # of states !

ν_0 = 1 topology (BiSb)



L.Fu, C.L.Kane PHYSICAL REVIEW B **76**, 045302 (2007)



s-wave proximity 2D boundary TI

$$H_{BdG} = \begin{pmatrix} \hat{h}_0(k) - \mu & \Delta \\ \Delta^\dagger & -\hat{h}_0^T(-k) + \mu \end{pmatrix}$$

$$\mathbf{\Psi} = [\psi_{k\uparrow}, \psi_{k\downarrow}, -\psi^\dagger_{-k\downarrow}, \psi^\dagger_{-k\uparrow}]$$

eigenvalues are: $\pm\sqrt{(\pm v|p| - \mu)^2 + \Delta^2}$

$$U\mathbf{\Psi} \ : [\phi_{kL}, \phi_{kR}, -[\phi_{-k\,\theta L}]^\dagger, [\phi_{-k\,\theta R}]^\dagger]$$

$$\phi_{kL} = \left(\psi_{k\uparrow} + e^{i\theta}\,\psi_{k\downarrow}\right), \quad \phi_{kR} = \left(e^{-i\theta}\,\psi_{k\uparrow} - \psi_{k\downarrow}\right)$$

$$[H_\Delta]_{\vec{k}} = -\Delta\left[e^{-i\theta_k}\,\phi^\dagger_{kL}\,[\phi_{-k\,\theta L}]^\dagger \; - e^{i\theta_k}\,\phi^\dagger_{kR}\,[\phi_{-k\,\theta R}]^\dagger\right] + h.c.$$

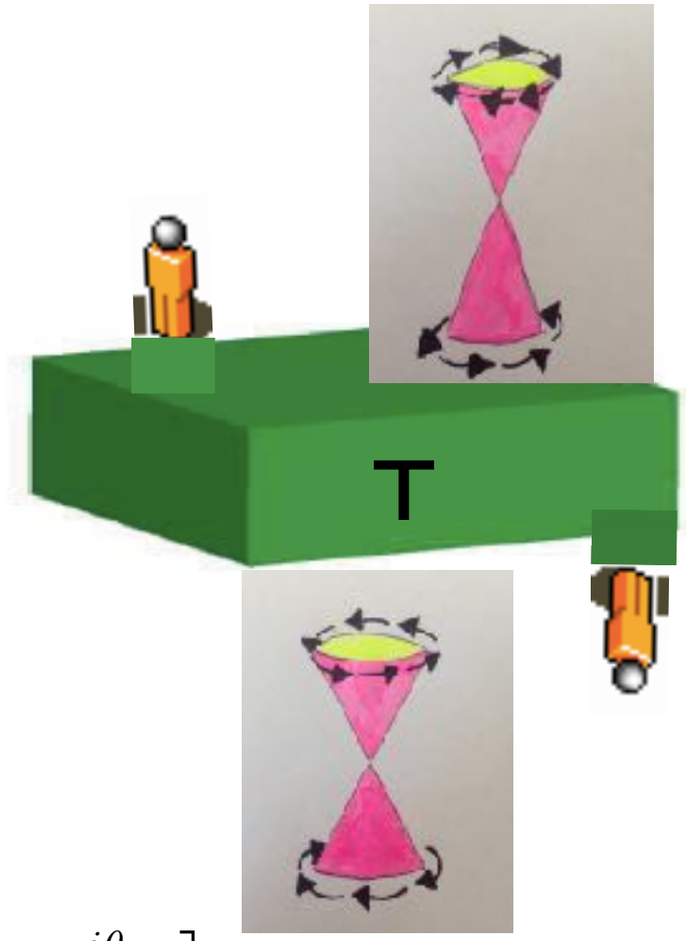
a $\Delta\,(p_x - ip_y)$ pairing appears

$$\Delta(z) = \langle\psi_{g\uparrow}\psi_{g\downarrow}\rangle = \langle\psi_{u\uparrow}\psi_{u\downarrow}\rangle$$

$$\Pi_L\,|a,+;k_\parallel\rangle \propto \begin{bmatrix} e^{-i\theta_{\vec{k}}}\begin{pmatrix} i \\ 1 \end{pmatrix} \\ 1\begin{pmatrix} 1 \\ i \end{pmatrix} \end{bmatrix} e^{-\int^z dz\,M(z)}; \quad \Pi_L\,|a,\Theta+;k_\parallel\rangle \propto -i\begin{bmatrix} \begin{pmatrix} i \\ 1 \end{pmatrix} \\ e^{i\theta_{\vec{k}}}\begin{pmatrix} 1 \\ i \end{pmatrix} \end{bmatrix} . e^{-\int^z dz\,M(z)}$$

3 D

exchange of helicities between the two surfaces:



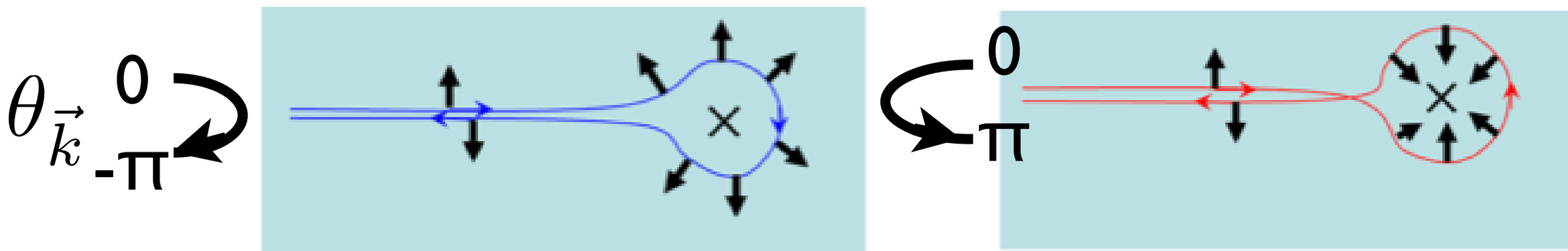
choosing one single helical boundary state $vk \sim \mu$

$$c_{\vec{k}} \equiv \begin{bmatrix} c_{\vec{k}\uparrow} \\ c_{\vec{k}\downarrow} \end{bmatrix} \rightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ e^{i\theta_k} \end{bmatrix} ; \quad -c_{-\vec{k}}{}^{\dagger} \equiv \begin{bmatrix} c_{-\vec{k}\downarrow}{}^{\dagger} \\ -c_{-\vec{k}\uparrow}{}^{\dagger} \end{bmatrix} \rightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\theta_k} \\ 1 \end{bmatrix} .$$

$$H^{new} = \frac{1}{2} \begin{pmatrix} c_{\vec{k}}{}^{\dagger} & -c_{-\vec{k}} \end{pmatrix} \begin{pmatrix} [vk-\mu] & \Delta e^{-i\theta_k} \\ \Delta e^{i\theta_k} & -[vk-\mu] \end{pmatrix} \begin{pmatrix} c_{\vec{k}} \\ -c_{-\vec{k}}{}^{\dagger} \end{pmatrix}$$

Read & Green 2000, Fu & Kane 2008

Absence of backscattering:



$$\varphi_{Berry} = -i \int_0^T dt \, \begin{pmatrix} 1 & -i\, e^{i\theta(t)} \end{pmatrix} \frac{1}{2} \frac{d}{dt} \begin{pmatrix} 1 \\ i\, e^{-i\theta(t)} \end{pmatrix} = - \int_0^T dt\, \dot{\theta} = \pm \frac{\pi}{2}$$

$$|\psi(t)\rangle' = |\circlearrowright\rangle = e^{i\frac{\pi}{2}} \, |\psi(0)\rangle \qquad \theta_{\vec{k}} \in (0, -\pi)$$

$$|\psi(t)\rangle'' = |\circlearrowleft\rangle = e^{-i\frac{\pi}{2}} \, |\psi(0)\rangle \qquad \theta_{\vec{k}} \in (0, \pi)$$

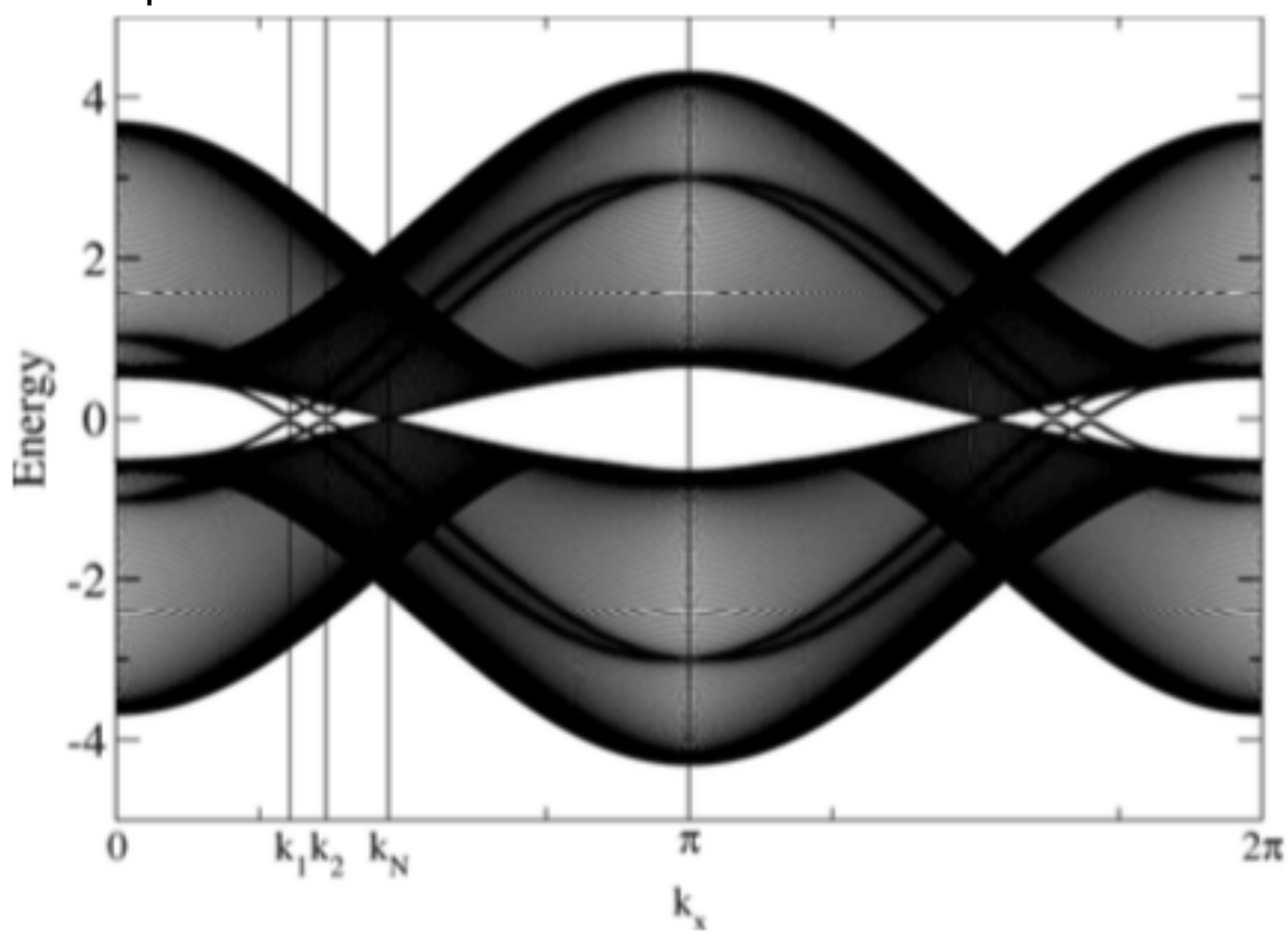
$$|\psi(t)\rangle = |\circlearrowleft\rangle + |\circlearrowright\rangle = \left(e^{i\frac{\pi}{2}} + e^{-i\frac{\pi}{2}}\right) |\psi(0)\rangle = \mathbf{0}$$

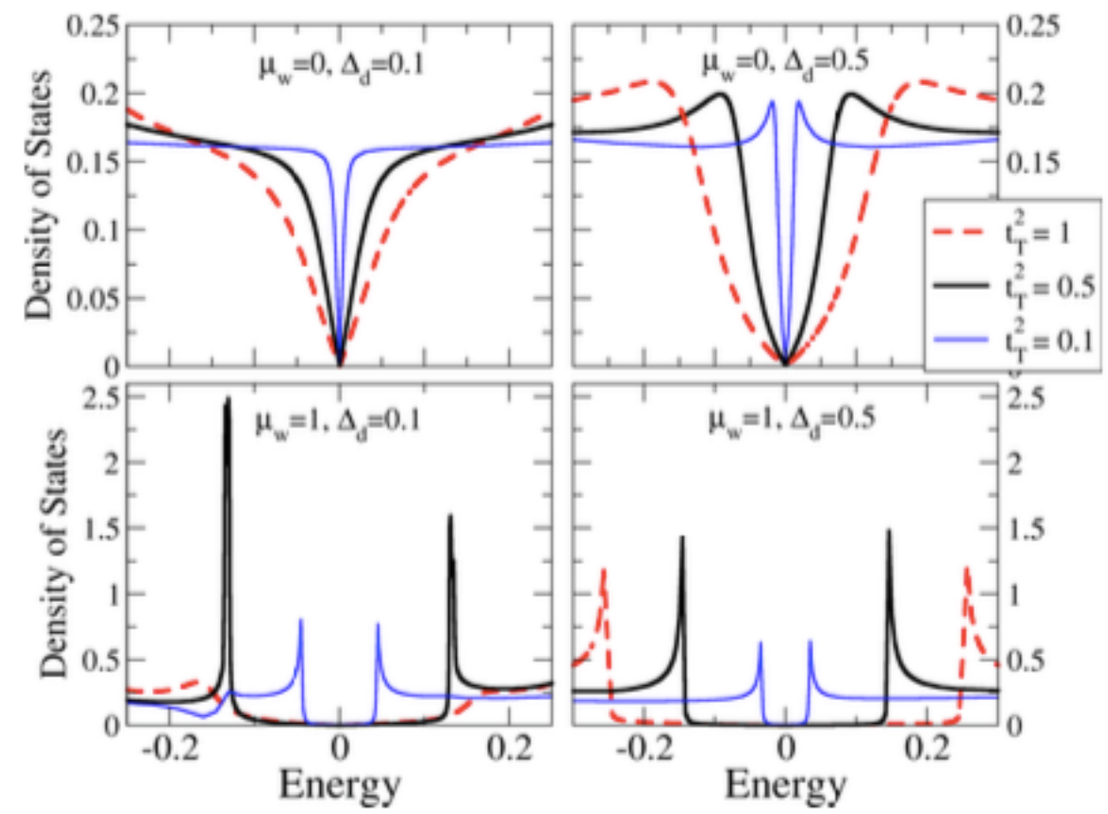
Proximity from a 2D d-wave conventional Superconductor to a 1D- wire with spin-orbit coupling (Numerical: tight-binding)

$$\mathcal{G}^w\left(i\omega, k_x\right) = \left[i\omega - Z(\xi^w_{k_x} - \delta\mu)\,\hat{\tau}_z - \hat{\Sigma}\left(i\omega, k_x\right)\right]^{-1}$$

$$\hat{\Sigma}\left(i\omega, k_x\right) = -i\omega(Z^{-1} - 1) - \delta\mu\,\hat{\tau}_z + \Delta_0(i\omega, k_x)(1 - Z)\hat{\tau}_x$$

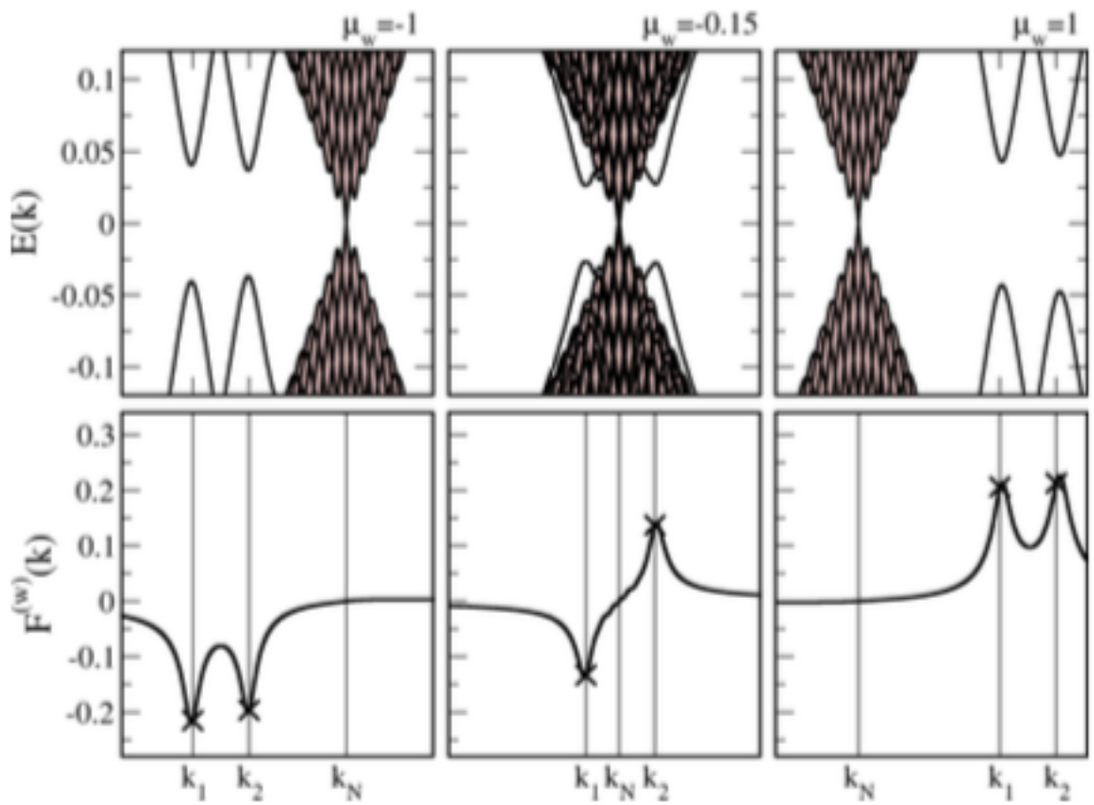
t_T=0.3, α=0.1, μ=-1.





$$F^{(w)}(k) = \frac{1}{2}\left\langle d_{k\uparrow} d_{-k\downarrow} - d_{k\downarrow} d_{-k\uparrow} \right\rangle$$

$$F^{(w)}(\ell) = \frac{1}{N_k} \sum_k F^{(w)}(k)\ \cos(k\ell)$$



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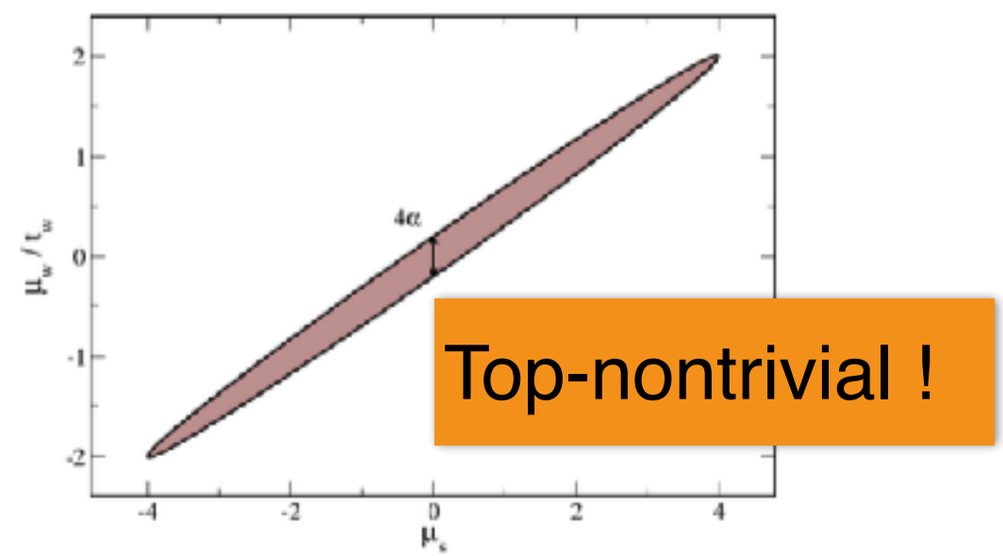
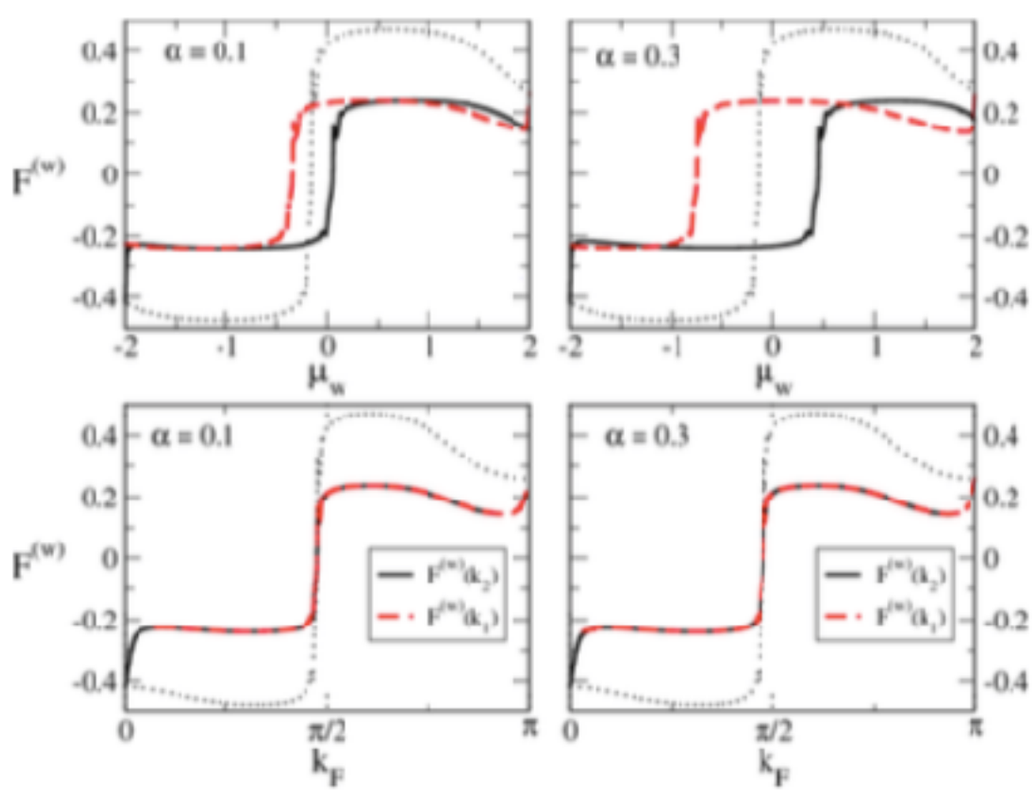
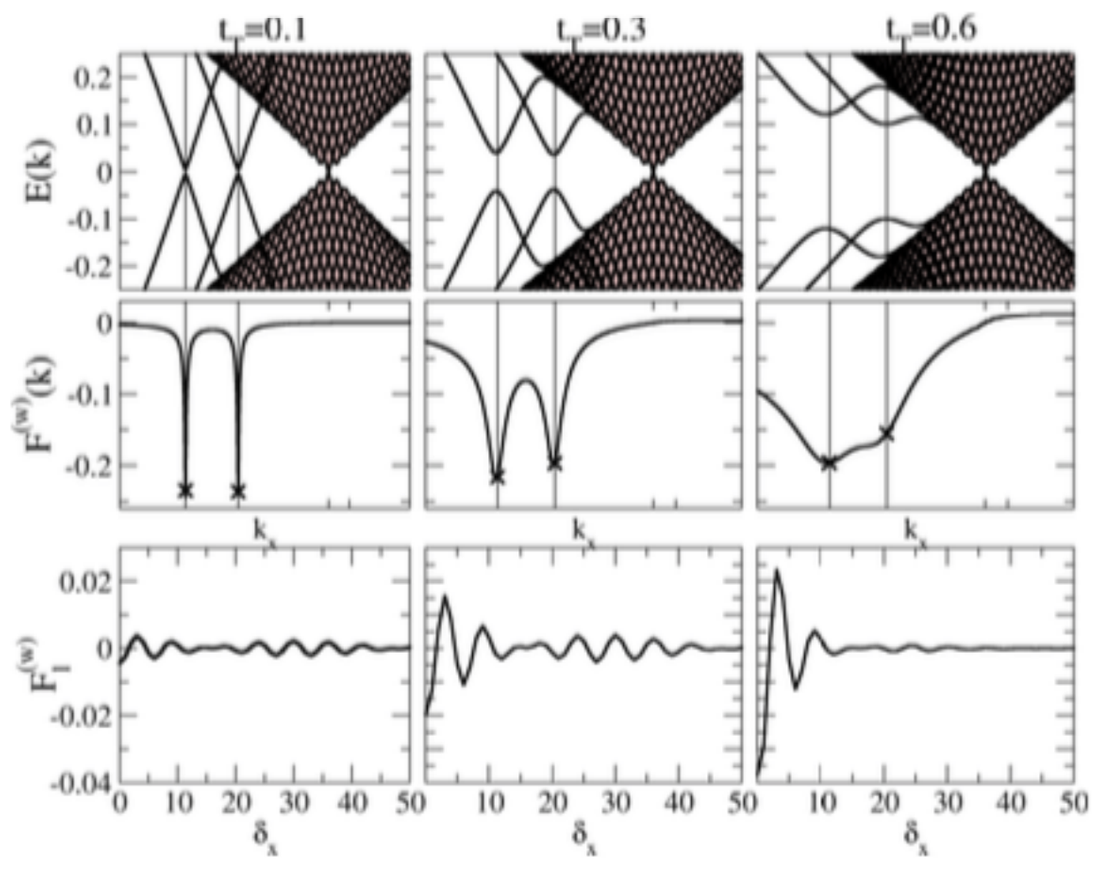


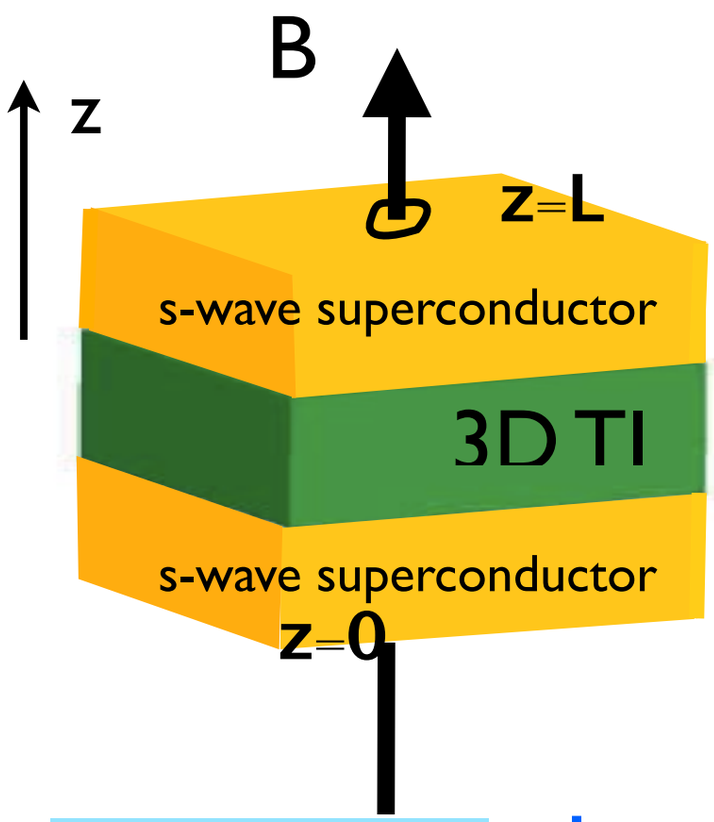
Top-nontrivial !





Vortex along z

Two spin polarized zero energy Majorana fermions bound at the interfaces with the superconductor



orbital angular momentum m=0 on surface z=0, but m=1 on surface z=L , due to the opposite chirality,

z=0	spin↑	m=0	j= 1/2
z=L	spin↓	m=1	j= 1/2

$j = m + s_z$

but both Majoranas have total m_J = 1/2

!

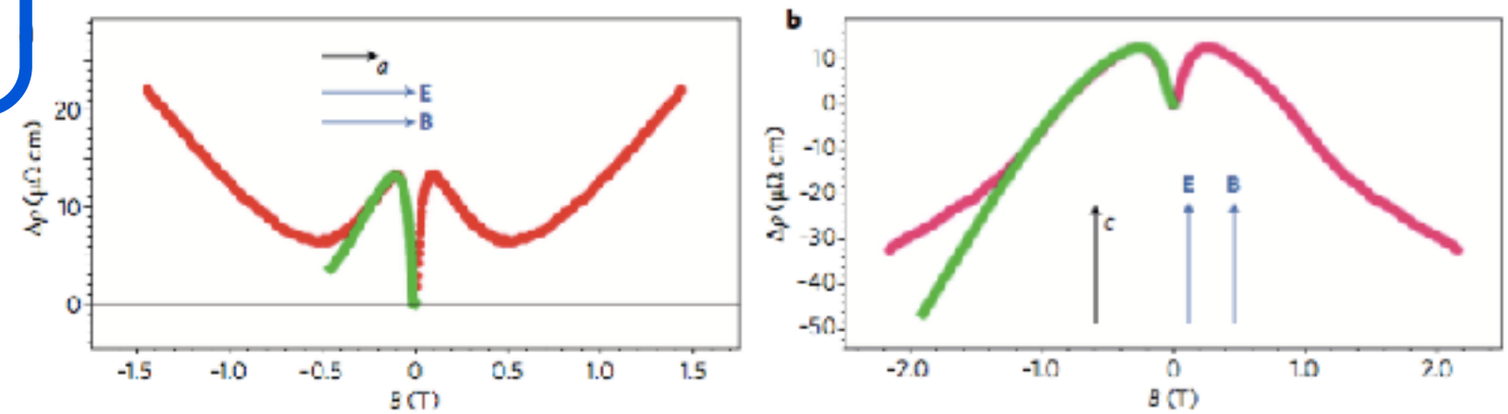
as if the vortex splits into two half vortices...

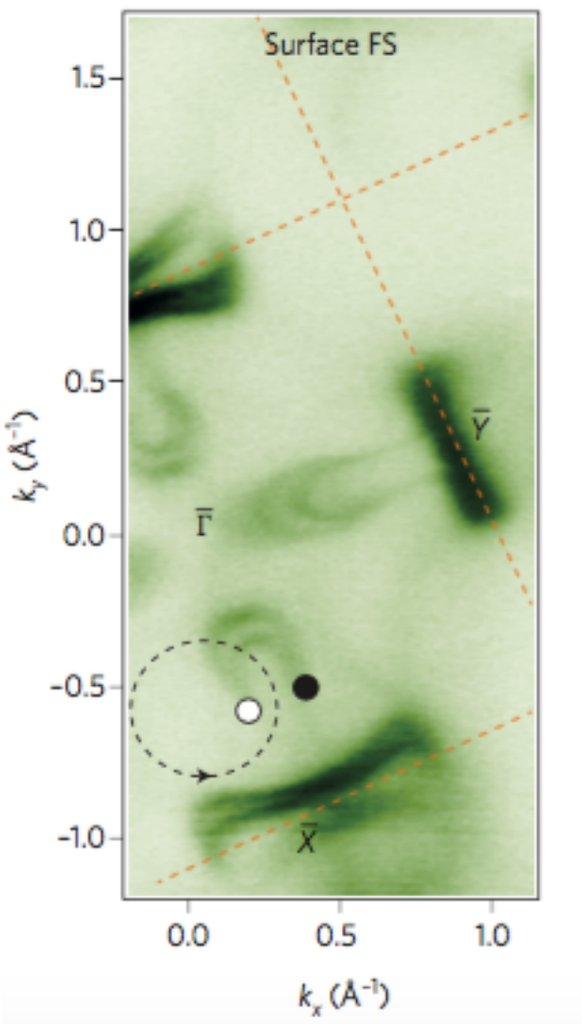
other bound qp levels:

$$E_n = n\,\omega_0 = n\frac{\Delta^2}{\epsilon_F} \qquad \mathbf{n \neq 0}$$

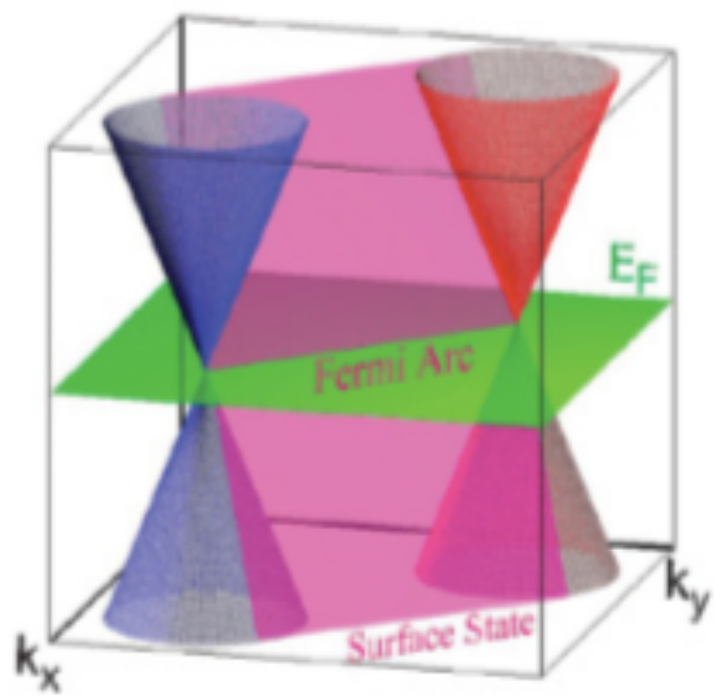
Weyl semimetals

$$P_3 \propto \vec{E} \cdot \vec{B}$$



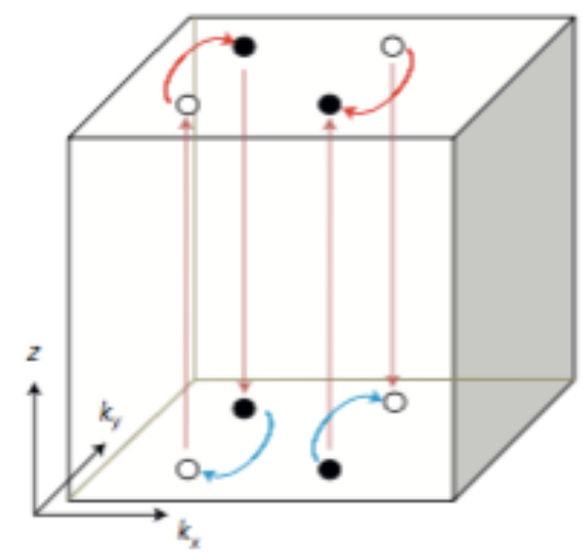


Breaking of inversion symmetry



Weyl nodes at E_F

of cones with opposite chirality



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3D-type IQHE without magnetic field

Summary:

- TI harbours one helical Dirac boundary state at each surface
  - s-wave proximity provides an effective *p-wave* pairing
  - spinless *p-wave* pairing localizes quasi-1D Majorana states at the edges
  - a vortex binds a Majorana fermion at top/bottom edges

addendum: wires, flakes and HTc superconductor:

- quasi 1D-Josephson Junction with $d_{x^2-y^2}$ sup-proximity in Kitaev simplified model chain
- intrinsic magnetic flux in aTI on a HTc tricrystal