08. Surface state of topological insulator

09. Weyl semimetal

10. Electromagnetic response of Weyl semimetal

11. Review of BCS theory

12. 1D p-wave superconductor

13. 2D p-wave superconductor

14. Superconductor with spin

15. Spinful p-wave superconductor with TRS

16. Periodic table

Homework (60%), term report (40%)

Surface state of topological insulator

A. Symmetry of Hamiltonian

B. Effective Hamiltonian of TI surface states

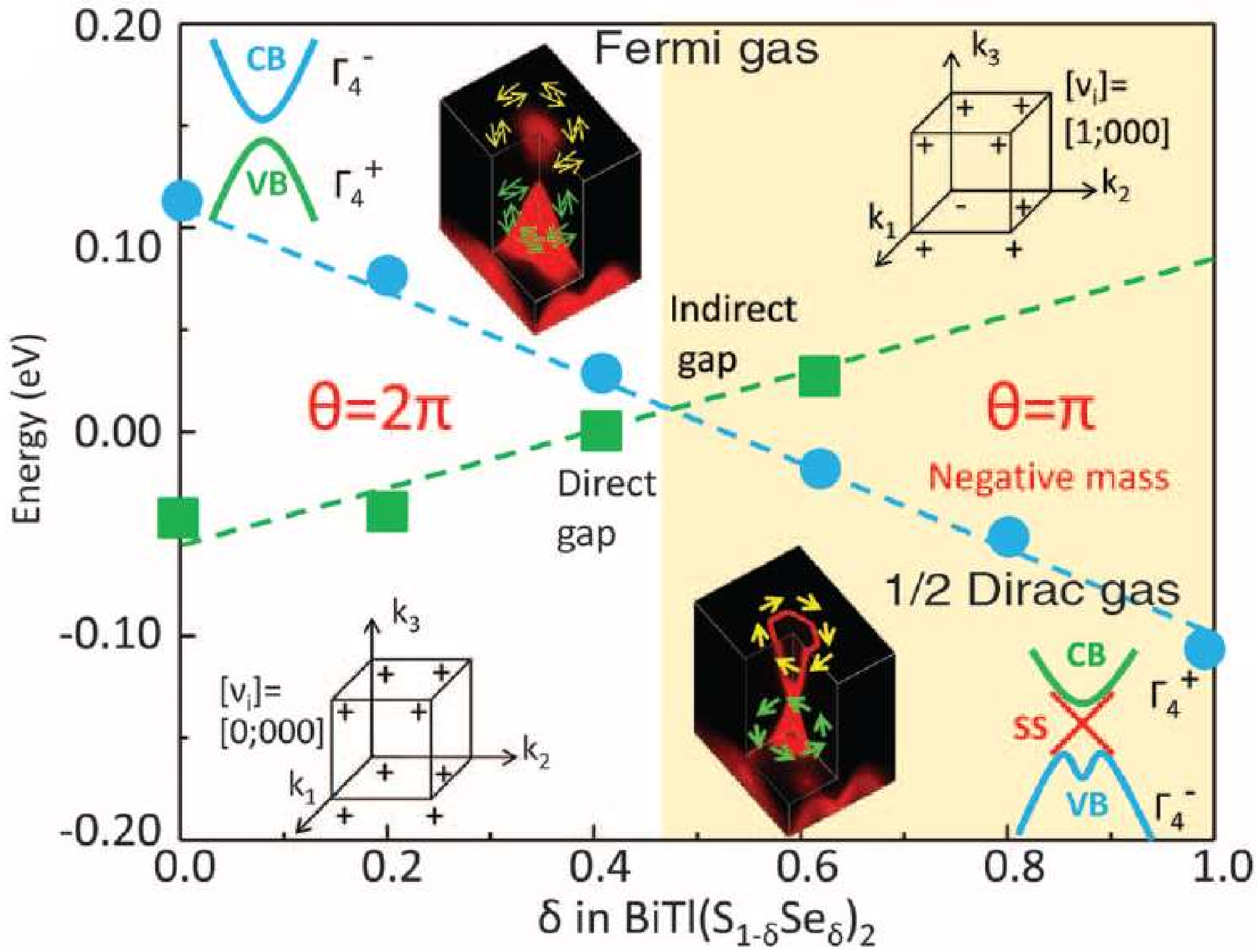
C. Berry curvature near level crossing

D. Electromagnetic response of surface state

   1. Magneto-electric coupling
   2. Axion electrodynamics
   3. Axion angle and Berry connection

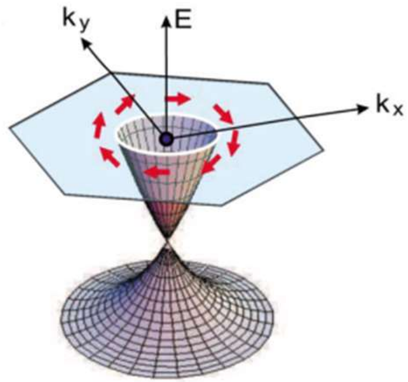
Band inversion, parity change, emergence of SS, and

spin-momentum locking all at once



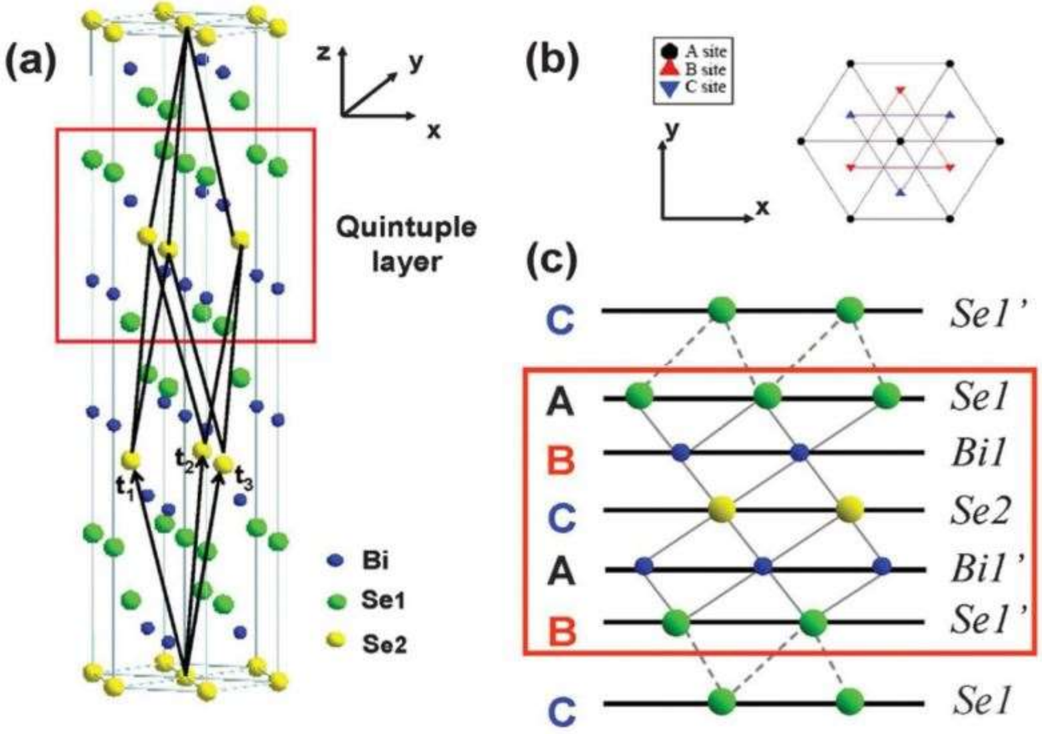
Low-energy Hamiltonian of SS

$$H_{SS} = \alpha(\vec{k} \times \vec{\sigma})_z$$



S.Y. Xu et al Science 2011

We now consider the surface of a topological insulator Bi_2Se_3



(a) Crystal structure of Bi2Se3.
(b) Top view of the (111)-surface.
(c) Side view of the layered structure.

There are 3 symmetries of surface atoms:

1. Time-reversal symmetry
2. A 3-fold rotation symmetry around the z-axis
3. A mirror symmetry w.r.t. the x-axis

We'll use symmetry to narrow down the form of low-energy surface-state Hamiltonian.

Here we only consider point-group symmetry (the symmetry operation that leaves a point fixed)

Suppose the Hamiltonian is,

$$H = \sum_{\alpha,\beta} H_{\alpha\beta}(\mathbf{k}) c^\dagger_\alpha(\mathbf{k}) c_\beta(\mathbf{k}),$$

- Invariance under a point-group symmetry transformation *g* requires that

$$\mathsf{U}_g \mathsf{H}(\mathbf{k}) \mathsf{U}_g^{-1} = \mathsf{H}(\mathsf{g}\mathbf{k}).$$

.e.g., for rotation, g is the usual 3x3 matrix, U_g is the matrix that rotates the bases of the Hamiltonian.

- Symmetry operators

1. $\Theta = i\sigma_y K \qquad \Theta^2 = -1$

2. $C_3 = e^{i\pi/3\sigma_z}$

3. $M = i\sigma_x \qquad M^2 = -1$

- Consider a 2-band model

$$\mathsf{H}(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & g(\mathbf{k}) \\ g^*(\mathbf{k}) & -h(\mathbf{k}) \end{pmatrix}$$

- Invariance under symmetry requires

$$\begin{aligned} \Theta\mathsf{H}(\mathbf{k})\Theta^{-1} &= \mathsf{H}(-\mathbf{k}), \\ C_3\mathsf{H}(k_\pm)C_3^{-1} &= \mathsf{H}(e^{\mp i2\pi/3}k_\pm), \\ M\mathsf{H}(k_\pm)M^{-1} &= \mathsf{H}(-k_\mp), \end{aligned}$$

1. time-reversal symmetry dictates that $h(-\mathbf{k}) = -h(\mathbf{k}), g(-\mathbf{k}) = -g(\mathbf{k})$.
2. Rotation symmetry gives

$$\begin{aligned} h(k_\pm) &= h(e^{\mp 2\pi i/3}k_\pm); \\ e^{i2\pi/3}g(k_\pm) &= g(e^{\mp 2\pi i/3}k_\pm). \end{aligned}$$

3. Mirror symmetry gives

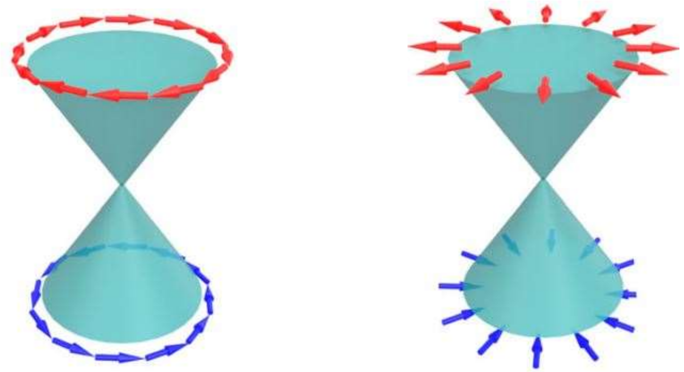
$$\begin{aligned} h(k_\pm) &= -h(-k_\mp); \\ g(k_\pm) &= g^*(-k_\mp). \end{aligned}$$

Effective Hamiltonian for 2D surface state

To linear order of the momentum, it is not difficult to see that $h(\mathbf{k}) = 0, g(\mathbf{k}) = ik_-$. Therefore,

$$\mathsf{H}(\mathbf{k}) = \varepsilon_0(k) + v(\sigma_x k_y - \sigma_y k_x).$$

- spin-momentum locking
  (Dirac cone with spin texture)

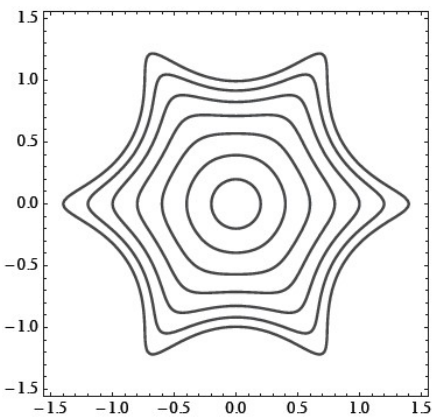


$H_{SS} = \alpha(\vec{k} \times \vec{\sigma})_z$ $\quad$ $H_{SS} = \alpha \vec{k} \cdot \vec{\sigma}$

- To the 3[rd] order of momentum (Fu PRL 2010)

$$H(\vec{k}) = \varepsilon_0(\vec{k}) I_{2\times 2}$$
$$+ v_k \left(k_x \sigma_y - k_y \sigma_x\right) + \frac{\lambda}{2}\left(k_+^3 + k_-^3\right)\sigma_z$$

$$\varepsilon_\pm(\mathbf{k}) = \varepsilon_0(k) \pm \sqrt{v_k^2 k^2 + \lambda^2 k^6 \cos^2(3\theta)}$$

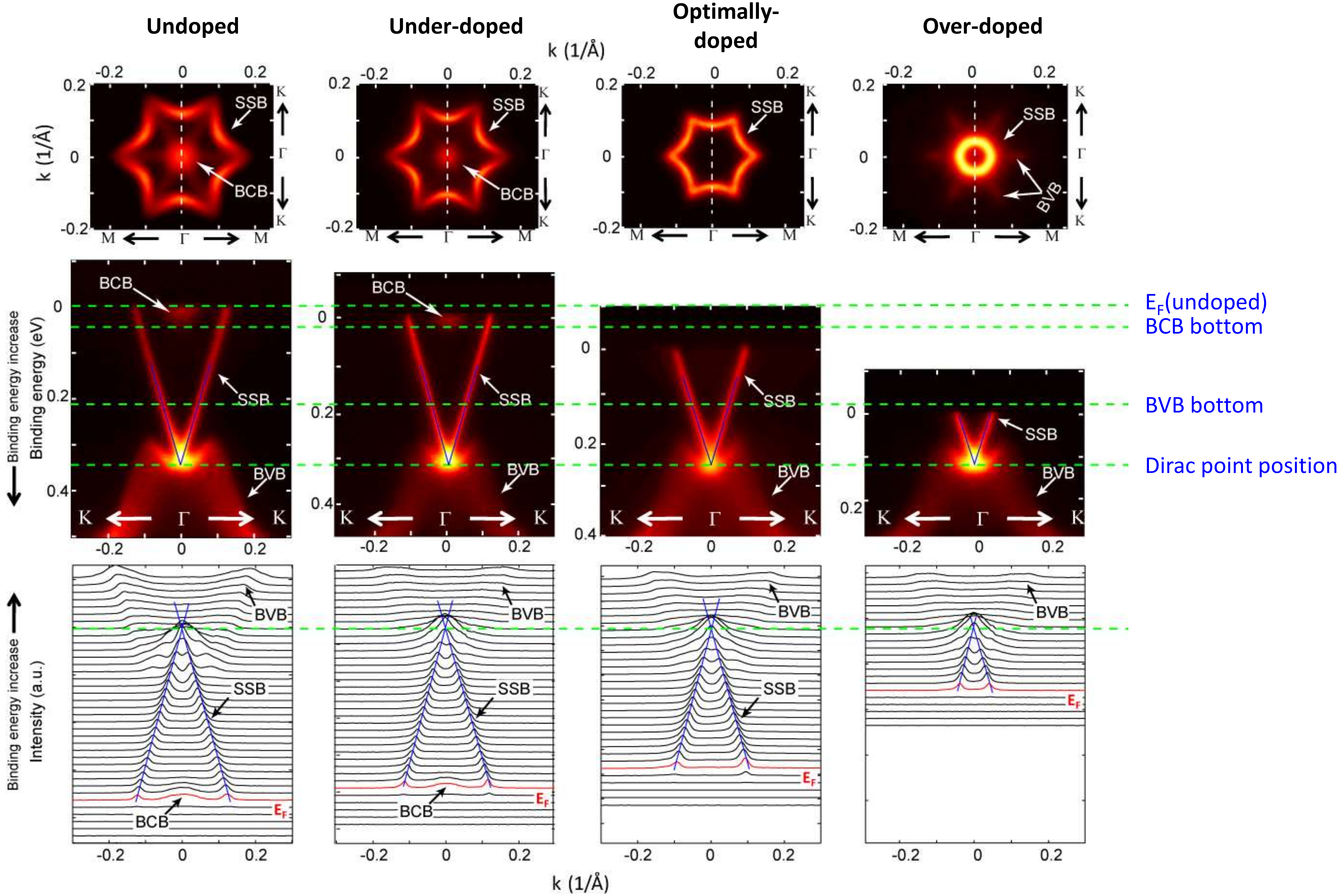


Warped Dirac cone

Fig from Krieger, Nat Comm 2024

Arpes experiment on Be_2Te_3 surface states, Shen group

Doping evolution of the FS and band structure



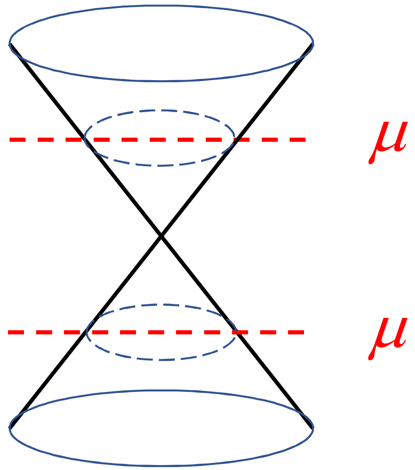
Berry curvature in surface state

Near a Dirac point

$$\mathrm{H}_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + O(k^2)$$

$$\gamma_C = \mp \frac{\Omega_C}{2} = \mp \pi$$

For a circle C around a DP



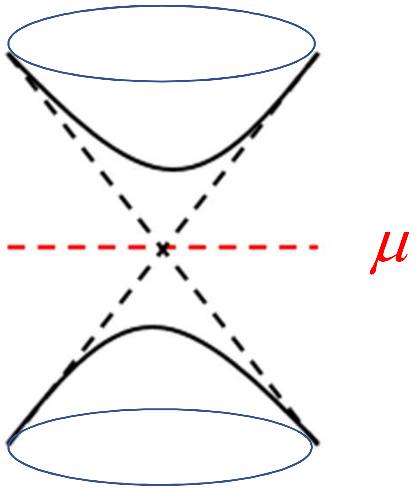
$$F_z^{\pm} = \mp \pi \delta^2(\mathbf{k})$$

$$\sigma_H = 0$$

Need to break TRS to have non-zero σ_H

- Open an energy gap by magnetization

$$\mathrm{H}_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + m\sigma_z$$

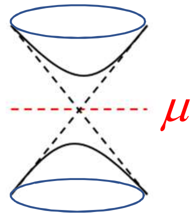


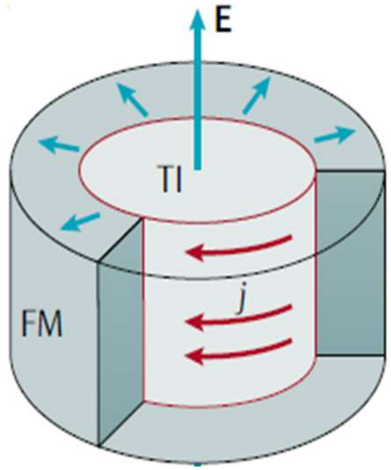
$$F_z^{\pm} = \mp \frac{\alpha^2 m}{2(m^2 + \alpha^2 k^2)^{3/2}}$$

$$\sigma_H = \frac{e^2}{h}\frac{1}{2\pi}\int d^2k F_z^- = \frac{1}{2}\frac{e^2}{h}$$

Half-integer QHE

Electromagnetic response of TI surface state





Surface state ～2 DEG

Half-integer QHE

• Hall current

$$J_H = \boxed{\frac{e^2}{2h}} E$$

• Induced magnetization

$$M = \frac{e^2}{2h} E$$

Magnetoelectric (ME) coupling

磁電耦合

• Symmetry of ME coupling

$$\alpha_{ij} = \left.\frac{\partial M_j}{\partial E_i}\right|_{\boldsymbol{B}=0} = \left.\frac{\partial P_i}{\partial B_j}\right|_{\boldsymbol{E}=0}$$

Electric field induces magnetization ↔

magnetic field induces polarization

$$P = \frac{e^2}{2h} B$$

The Lagrangian density for Maxwell theory (see, e.g., Jackson)

$$L_0 = \frac{\varepsilon_0}{2}\left(E^2 - c^2 B^2\right) - \rho\phi + \vec{J}\cdot\vec{A}$$ (SI, latex note uses cgs)

- To have the ME coupling, we need to add a term,

$$L_{axion} = \frac{e^2}{2h}\vec{E}\cdot\vec{B} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\alpha\frac{\Theta}{\pi}\vec{E}\cdot\vec{B}$$

also called Axion coupling

軸子

fine structure constant

$$\alpha = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}$$

- Axion angle

$$\Theta = \begin{cases} \pi \text{ for TI} \\ 0 \text{ for trivial} \end{cases}$$

Cr_2O_3: θ ~ π/24 (TRS is broken)

- From the Euler-Lagrange eq. of motion, we get the Maxwell equations (see latex note for derivation)

$$\frac{\partial \mathcal{L}_{EM}}{\partial A_\nu} - \partial_\mu \frac{\partial \mathcal{L}_{EM}}{\partial(\partial_\mu A_\nu)} = 0$$

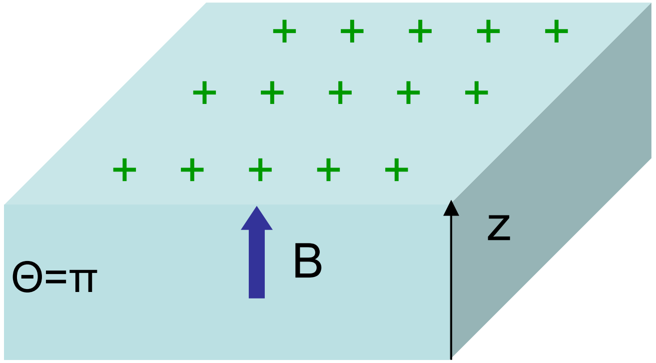
$$L_{EM} = L_0 + L_{axion}$$

Maxwell eqs with axion coupling (suppose ε, μ are constants)

$$\begin{cases} \nabla\cdot\left(\vec{E}+\alpha\frac{\Theta}{\pi}c\vec{B}\right)=\frac{\rho}{\varepsilon} \\ \nabla\times\left(\vec{B}-\alpha\frac{\Theta}{\pi c}\vec{E}\right)=\mu\vec{J}+\frac{\partial}{c^2\partial t}\left(\vec{E}+\alpha\frac{\Theta}{\pi}c\vec{B}\right) \\ \nabla\cdot\vec{B}=0 \\ \nabla\times\vec{E}=-\frac{\partial}{\partial t}\vec{B} \end{cases}$$

- B-induced charge

$$\rho_\Theta=c\alpha\varepsilon\delta(z)B_z$$



Effective charge and effective current

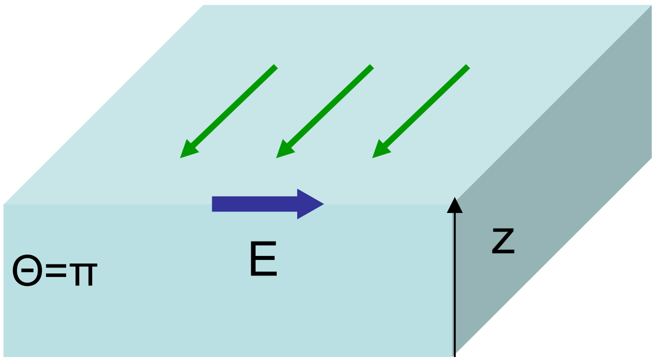
$$\begin{cases} \nabla\cdot\vec{E}=\frac{\rho+\rho_\Theta}{\varepsilon} \\ \rho_\Theta=-\frac{c\alpha\varepsilon}{\pi}\nabla\cdot\left(\Theta\vec{B}\right) \\ \nabla\times\vec{B}=\mu\left(\vec{J}+\vec{J}_\Theta\right)+\frac{1}{c^2}\frac{\partial\vec{E}}{\partial t} \\ \vec{J}_\Theta=\frac{\alpha}{\pi c\mu}\nabla\times\left(\Theta\vec{E}\right)+\frac{\alpha}{\pi c\mu}\frac{\partial}{\partial t}\left(\Theta\vec{B}\right) \end{cases}$$

B-induced charge

E-induced current

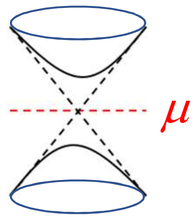
- E-induced current

$$\vec{J}_\Theta=-\frac{\alpha}{c\mu}\delta(z)\hat{z}\times\vec{E}\rightarrow\sigma_{xy}=\frac{1}{2}\frac{e^2}{h}$$



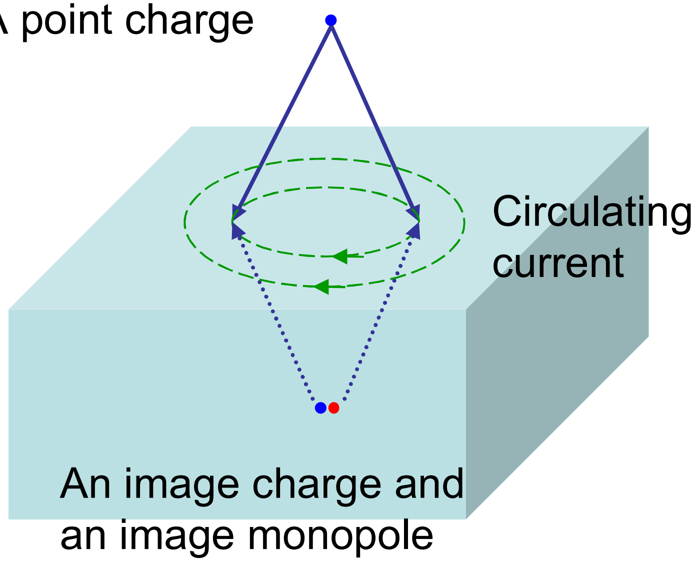
½ QH effect and theta=pi are basically the same

Axion effect



Static:

- Half-integer QHE
- Magnetic monopole in TI
- …



Qi, Hughes, and Zhang, Science 2009

Dynamic:

- Snell's law
- Fresnel formulas
- Brewster angle
- Faraday effect
- Kerr effect
- …

½ QH effect ↔ axion effect

Aka Topological Magnetoelectric Effect (TME)

General form of magneto-electric susceptibility $\chi_{ij} = \frac{\partial M_j}{\partial E_i} = \frac{\partial P_i}{\partial B_j}$

$$\chi_{ij} = \tilde{\chi}_{ij} + \chi_\theta \delta_{ij}$$

$$\chi_\theta = \frac{e^2}{2hc}\frac{\theta}{\pi}$$

Berry connection

$$[\mathsf{A}_a(\mathbf{k})]_{nn'} = i\langle u_{n\mathbf{k}}|\frac{\partial}{\partial k_a}|u_{n'\mathbf{k}}\rangle$$

$$\theta = \frac{1}{4\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}_a\partial_b\mathsf{A}_c - \frac{2i}{3}\mathsf{A}_a\mathsf{A}_b\mathsf{A}_c\right)$$

The integrand is called the Chern-Simon form.

Q: Why Chern-Simon form (if you have heard of it)?

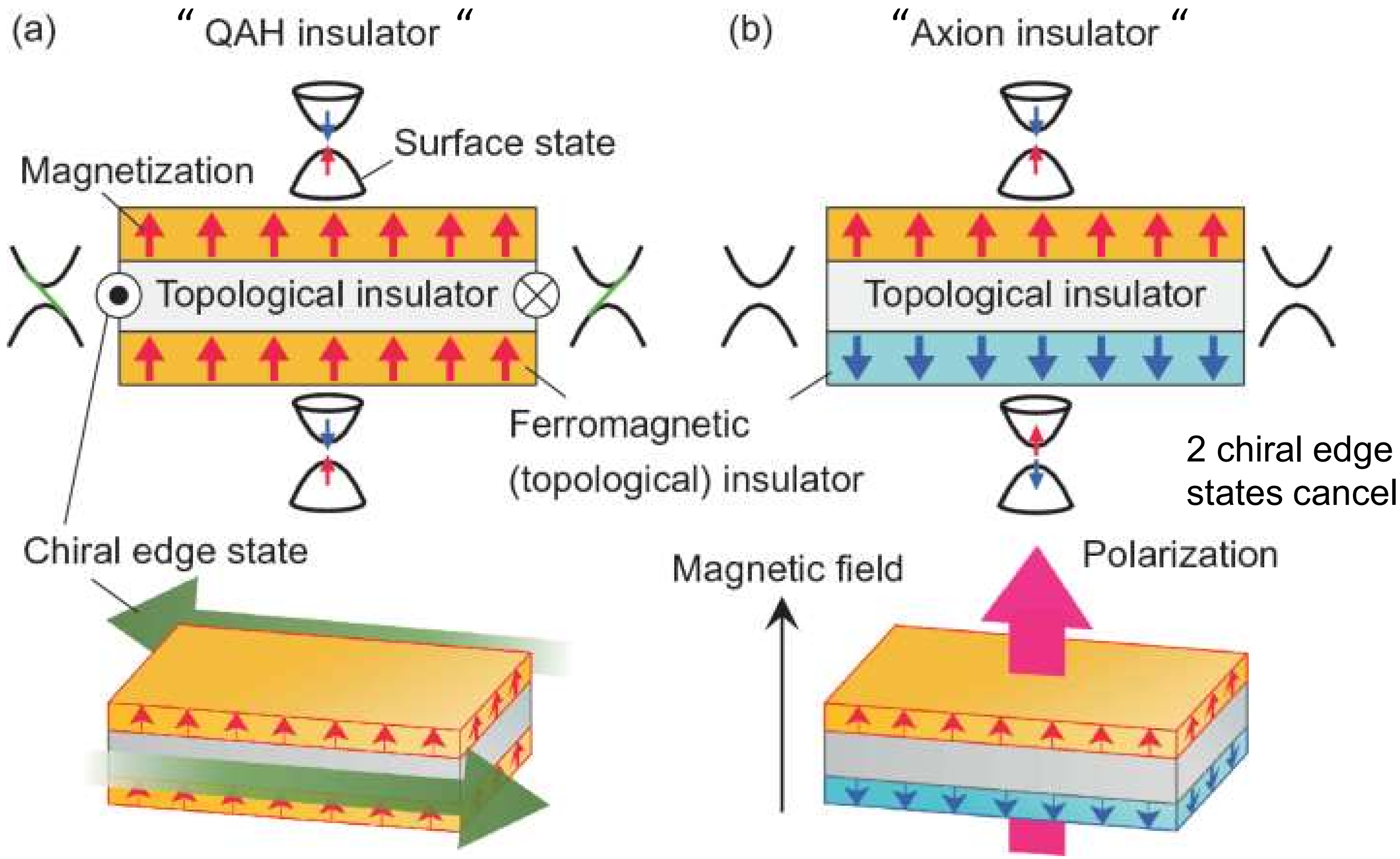
A: Close connection between 3D TI and 4D QHE

It can be proved that, with TRS, the axion angle is defined only up to $2\pi w, w \in Z$. (Wang et al, New J. Phys. 2010)

Θ changes sign under TR, so with TRS, Θ can only be 0 or π

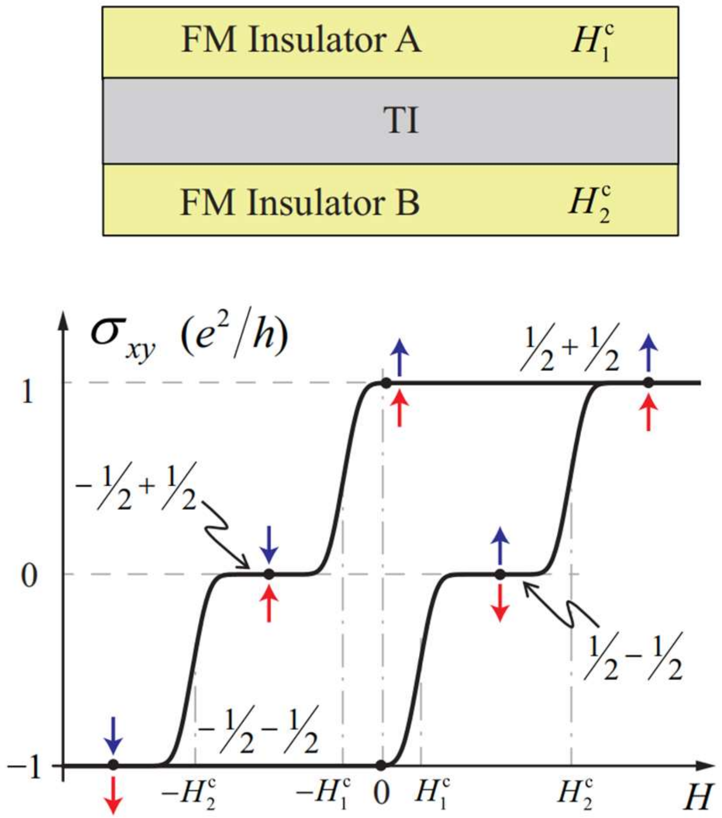
Microscopic expression of χ_{ij} from 2nd order perturbation theory:

Essin et al, PRB 2010; Malashevich et al, NJP 2010

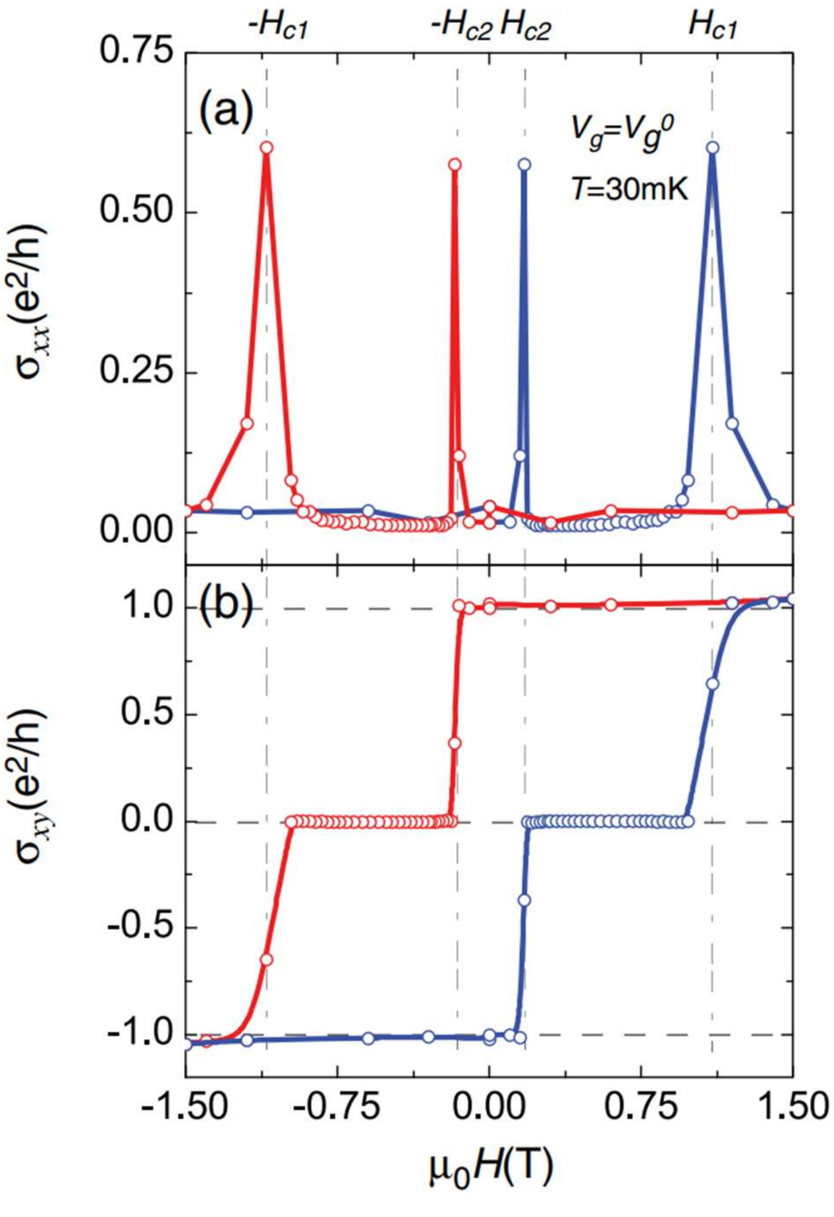


Dynamic TME possible.

Anything interesting?



Wang et al, PRB 2015



Mogi et al, Nat Mat 2017
Xiao et al, PRL 2018