@ Oka group, group seminar, April, 18, 2025

Electromagnetic Responses of 3D Topological Insulators and Axion Electrodynamics in Condensed Matter Systems

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- This talk is based on my Bacheor Thesis at Tada group in Hiroshima University.
- ✓ My bacheor thesis written in Japanese can be found in my HP. Scan the right QR code \rightarrow .



Outline

This talk consists of three parts.

Background

Electromagnetic Responses of 3D Topological Insulators

Axion Electrodynamics in Topological Materials

This talk is mainly based on two papers: Qi, Hughes, and Zhang, Phys. Rev. B, (2008) and Sekine and Nomura, J. Appl. Phys., (2021)

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Background

 In 1950s, Ginzburg and Landau developed the standard theory for phases and phase transitions.
 → Very Successful

Xiao-Gang Wen, Rev. Mod. Phys., (2017)

- However, in 1980s, Quantum Hall Effect (QHE) was discovered as a first example of Topological Phases.
 K. v. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett., (1980)
- In 2005, Kane and Mele proposed Topological Insulators (TIs) protected by time reversal symmetry.

Bulk \rightarrow Energy Gap = like an Insulator Edge \rightarrow No Energy Gap = like a Metal

C. L. Kane and E. J. Mele, Phys. Rev. Lett., (2005)

C. L. Kane and E. J. Mele, Phys. Rev. Lett., (2005)

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Background

 In 2006 and 2007, Fu, Kane and Mele developed a basic theory of topological insulators including the topological band theory and 3D topological Insulators.

> Liang Fu and C. L. Kane, *Phys. Rev. B*, (2006) Liang Fu and C. L. Kane, *Phys. Rev. B*, (2007) Liang Fu, C. L. Kane, and E. J. Mele, *Phys. Rev. Lett.*, (2007)

- In 2008, Qi, Hughes and Zhang construct a topological field theory that describe topological responses of TIs.
 → In 3D TIs, effective action is equivalent to Axion Electrodynamics.
 Qi, Hughes, and Zhang, Phys. Rev. B, (2008)
- There are some theoretical proposal that potentially realize Axion electrodynamics in materials.

Sekine and Nomura, J. Appl. Phys., (2021)

Notations

 $\mu, \nu, \rho, \sigma = 0, 1, 2, 3, \cdots$: Indices for space-time

 $i, j, k, l = 1, 2, 3, \cdots$: Indices for space

Natural units: $\hbar = c = e = 1$ (restored when necessary)

Minkowski metric: $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1, \cdots)$

 $\alpha,\beta=1,2,3,\cdots$: Band Indices

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Electromagnetic Responses of 3D TIs

- 1. Quantum Hall Effect and Chern-Simons gauge theories
- 2. Effective Action of 3D Topological Insulators
- 3. Topological Electromagnetic Response
 - 3.1. Surface Half-integer Quantum Hall Effect3.2. Topological Magnetoelectric Effect

QHE and Chern-Simons gauge theories

First, we consider the effecvie action of QHE

$$S_{\rm CS}^{(2+1)} = \frac{Ch_1}{4\pi} \int d^2x dt \ \epsilon^{\mu\nu\rho} A_{\mu} \partial_{\nu} A_{\rho}$$

 $Ch_1 = \frac{1}{4\pi} \int d^2k \ \epsilon^{ij} \operatorname{Tr}[f_{ij}]$ is the first Chern number

 A_{μ} is the U(1) gauge field f_{ij} is the Berry curvature

Topological Response (= Hall current) can be calculated as

$$j^{\mu} = \frac{\delta S_{\rm CS}^{(2+1)}}{\delta A_{\mu}} = \frac{Ch_1}{2\pi} \epsilon^{\mu\nu\rho} \partial_{\nu} A_{\rho} = \sigma_{\rm H} \epsilon^{\mu\nu\rho} \partial_{\nu} A_{\rho}$$

QHE and Chern-Simons gauge theories

Next, we consider the 4D generalized QHE

Zhang and Hu, Science, (2001) Bernevig et. al., Ann. Phys., (2002)

- Chern-Simons gauge theory can be defined in odddimenstion space-time.
- (2+1)-d QHE can be generalized to (4+1)-d.
- 4D QHE is time reversal invariant.

QHE and Chern-Simons gauge theories

The effecvie action of the 4D generalized QHE:

$$S_{\rm CS}^{4+1} = \frac{Ch_2}{24\pi^2} \int d^4x dt \ \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau$$

$$Ch_{2} = \frac{1}{32\pi^{2}} \int d^{4}k \ \epsilon^{ijkl} \operatorname{Tr} \left[f_{ij} f_{kl} \right] \quad : \text{Second Chern number}$$
$$f_{ij}^{\alpha\beta} = \partial_{k_{i}} a_{j}^{\alpha\beta} - \partial_{k_{j}} a_{i}^{\alpha\beta} + i [a_{i}, a_{j}]^{\alpha\beta} : \text{Berry curvature}$$
$$a_{i}^{\alpha\beta} = -i \left\langle u_{\alpha, \mathbf{k}} | \partial_{k_{i}} | u_{\beta, \mathbf{k}} \right\rangle \qquad : \text{Berry connection}$$

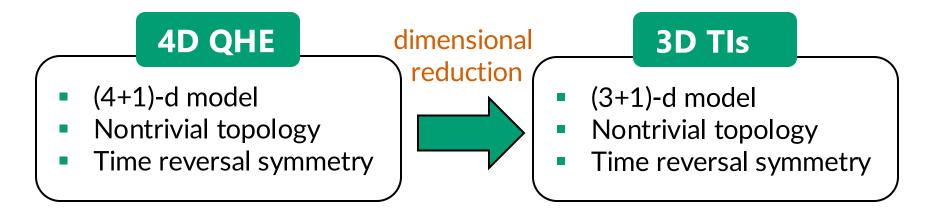
Topological Response (= Hall current) can be calculated as

$$j^{\mu} = \frac{\delta S_{\rm CS}^{(4+1)}}{\delta A_{\mu}} = \frac{Ch_2}{8\pi^2} \epsilon^{\mu\nu\rho\sigma\tau} \partial_{\nu} A_{\rho} \partial_{\sigma} A_{\tau}$$

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 Here, we derive the effective action of 3D TIs by dimensional reduction.

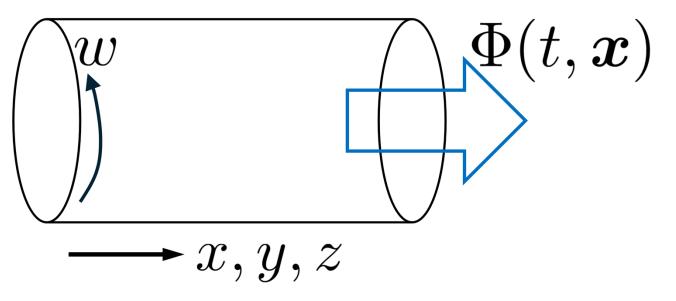


Effective action \rightarrow (4+1)-d Chern-Siomons gauge theory Effective action \rightarrow ???

We consider the 4D QHE on generalized cylinder.

Gauge field configurations: $A_{\mu} = (A_0, A_1, A_2, A_3, \Phi(t, \boldsymbol{x})/L_w)$, which do not depend on the *w* direction.

Integrate action out with respect to w direction and $L_w
ightarrow 0$



Effective action of 4D QHE can be calculated as

$$S_{\rm CS}^{4+1} = \frac{Ch_2}{24\pi^2} \int d^4x dt \ \epsilon^{\mu\nu\rho\sigma\tau} A_{\mu} \partial_{\nu} A_{\rho} \partial_{\sigma} A_{\tau}$$
$$= \frac{1}{8\pi^2} \int d^3x dt \ \theta(t, \boldsymbol{x}) \epsilon^{\mu\nu\rho\sigma} \partial_{\mu} A_{\nu} \partial_{\rho} A_{\sigma}.$$

We define the theta field or Axion field as

$$\theta(t, \boldsymbol{x}) = Ch_2 \Phi(t, \boldsymbol{x}) = -\frac{1}{4\pi} \int d^3k \ \epsilon^{ijk} \operatorname{Tr} \left[a_i \partial_j a_k + \frac{2}{3} i a_i a_j a_k \right].$$

Time reversal symmetry constraint quantizes Axion field.

$$\theta(t, \boldsymbol{x}) = 0, \pi \pmod{2\pi}$$

✓
$$\theta = 0$$
 → Trivial Insulators.
✓ $\theta = \pi$ → Strong Topological Insulators.

Therefore, effective action of 3D TIs are given by

$$S_{3D} = \frac{e^2}{8\pi^2 \hbar c} \int d^3 x dt \ \theta(t, \boldsymbol{x}) \epsilon^{\mu\nu\rho\sigma} \partial_\mu A_\nu \partial_\rho A_\sigma$$
$$= \frac{e^2}{4\pi \hbar c} \int d^3 x dt \ \boldsymbol{E}(t, \boldsymbol{x}) \cdot \boldsymbol{B}(t, \boldsymbol{x}).$$
Qi, Hughes, and Zhang, Phys. Rev. B, (2008)

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• Now we have two kinds of strong \mathbb{Z}_2 topological invariants.

 $\theta(t, \boldsymbol{x}) = 0, \pi \pmod{2\pi}$ From Topological field theory $(-1)^{\nu_0} = \prod_{n_1, n_2, n_3 = 0, 1} \delta(\Lambda_{i=(n_1 n_2 n_3)})$ From Topological band theory

These strong \mathbb{Z}_2 topological invariants are equivalent!!!.

Wang, Qi, and Zhang, New J. Phys., (2010)

 ν_0 : Can be easily computed θ : Directly observable in response coefficients

Surface Half-integer Quantum Hall Effect

- We consider the situation where z < 0 is the topological insulator and z > 0 is the trivial vaccum.
- Axion field: $\partial_z \theta(t, \boldsymbol{x}) = \pi \delta(z)$
- Effective action at surface: $S_{\text{surface}} = \frac{1}{8\pi} \int dx dy dt \ \epsilon^{\mu\nu\rho} A_{\mu} \partial_{\nu} A_{\rho}$

Then, the current at surface z = 0 is

$$j^{\mu} = \frac{\delta S_{\text{surface}}}{\delta A_{\mu}} = \frac{1}{2} \frac{e^2}{h} \epsilon^{\mu\nu\rho} \partial_{\nu} A_{\rho}$$

$$\begin{array}{l} \textbf{Topological}\\ \textbf{Insulators}\\ \theta=\pi \end{array} \quad \begin{array}{l} \textbf{Trivial}\\ \textbf{Vacuum}\\ \theta=0 \end{array}$$

z < 0 z > 0

Half quantized Hall conductance!!!

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Surface Half-integer Quantum Hall Effect

- Physically, the surface half-integer quantum Hall effect originates from a single Dirac cone at surface.
- Consider the effective Hamiltonian of 3D TIs at surface with magnetic impurities. <u>Zhang, et al., Nat. Phys., (2009)</u>

$$H_{\text{surface}}(k_x, k_y) = \hbar v_{\text{F}}(k_y \sigma_x - k_x \sigma_y) + \boldsymbol{m} \cdot \boldsymbol{\sigma}$$

H)

Topological Magnetoelectric Effect

• Total effective actions in 3D TIs are

$$S_{\text{tot}} = S_{\text{Maxwell}} + S_{3D}$$

= $\int d^4x \left[-\frac{1}{16\pi} F^{\mu\nu} F_{\mu\nu} + \frac{1}{2} F_{\mu\nu} \mathcal{P}^{\mu\nu} - \frac{1}{c} j^{\mu} A_{\mu} \right]$
+ $\frac{e^2}{8\pi^2 \hbar c} \int d^3x dt \ \theta(t, \mathbf{x}) \epsilon^{\mu\nu\rho\sigma} \partial_{\mu} A_{\nu} \partial_{\rho} A_{\sigma}$

 $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$: Field strength tensor

 $\mathcal{P}^{0i} = P_i, \mathcal{P}^{ij} = \epsilon^{ijk} M_k$: Electric polarization, Magnetization

> Equation of motion
$$\Box$$
 $\frac{\delta S_{\text{tot}}}{\delta A_{\mu}} = 0$

Topological Magnetoelectric Effect

• We derive the Modified Maxwell Equations in 3D TIs.

$$\nabla \cdot \boldsymbol{D} = 4\pi\rho$$

$$\nabla \times \boldsymbol{H} - \frac{1}{c} \frac{\partial \boldsymbol{D}}{\partial t} = \frac{4\pi}{c} \boldsymbol{j} \quad \alpha : \text{Fine structure constant}$$

$$\nabla \cdot \boldsymbol{B} = 0$$

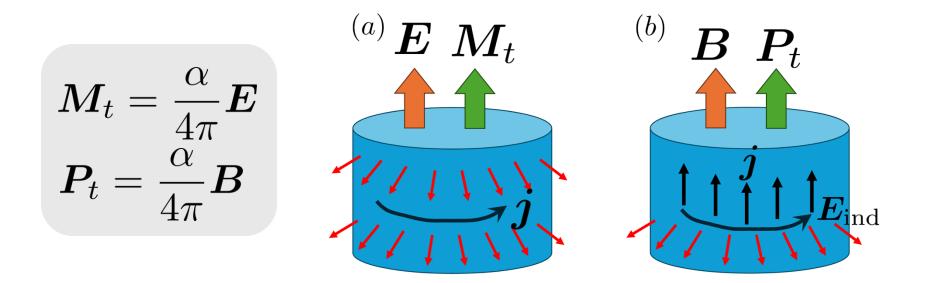
$$\nabla \times \boldsymbol{E} + \frac{1}{c} \frac{\partial \boldsymbol{B}}{\partial t} = 0$$

$$\boldsymbol{D} = \boldsymbol{E} + 4\pi\boldsymbol{P} + \frac{\alpha}{\pi}\theta\boldsymbol{B} = \epsilon\boldsymbol{E} + \frac{\alpha}{\pi}\theta\boldsymbol{B}$$

$$\boldsymbol{H} = \boldsymbol{B} - 4\pi\boldsymbol{M} + \frac{\alpha}{\pi}\theta\boldsymbol{E} = \frac{\boldsymbol{B}}{\mu} + \frac{\alpha}{\pi}\theta\boldsymbol{E}$$

Topological Magnetoelectric Effect

 Physically, the topological magnetoelectric effect originates from a surface half quantized hall current.



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Axion Electrodynamics in Topological Materials

- 1. Chiral Anomaly
- 2. Derivation of Effective Action of 3D TIs
- 3. Dynamical Axion Fields
- 4. Weyl Semimetals

Axion Electrodynamics in Topological Materials

• The action for Axion electrodynamics

$$S_{\theta} = \frac{e^2}{8\pi^2} \int d^3x dt \ \theta(t, \boldsymbol{x}) \epsilon^{\mu\nu\rho\sigma} \partial_{\mu} A_{\nu} \partial_{\rho} A_{\sigma}$$
$$= \frac{e^2}{32\pi^2} \int d^3x dt \ \theta(t, \boldsymbol{x}) \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}$$

• Actually, S_{θ} originates from the chiral anomaly in (3+1)-d.

First, we review the chiral anomaly.

Chiral Anomaly

• The action for Dirac field in (3+1)-d with U(1) gauge fields

$$S[\bar{\psi},\psi,A_{\mu}] = \int d^4x \ \bar{\psi}[i\gamma^{\mu}D_{\mu} - m]\psi$$

 $D_{\mu} = \partial_{\mu} - ieA_{\mu}$: Covariant derivative

Chira transformation:
$$\psi \to \psi' = e^{i\alpha\gamma^5}\psi$$

 $\bar{\psi} \to \bar{\psi}' = \bar{\psi}e^{i\alpha\gamma^5}$

• In m = 0, the action has chiral symmetry

$$S\left[\bar{\psi},\psi,A_{\mu}\right] = S\left[\bar{\psi}',\psi',A_{\mu}\right]$$

Chiral Anomaly

• In quantum mechanics, we require that the partition function is invariant under the chrial transformation.

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \ e^{iS\left[\bar{\psi},\psi,A_{\mu}\right]} = \int \mathcal{D}\bar{\psi}'\mathcal{D}\psi' \ e^{iS\left[\bar{\psi}',\psi',A_{\mu}\right]}$$

- The integral measure transforms as $\mathcal{D}\bar{\psi}'\mathcal{D}\psi' = J(\alpha)\mathcal{D}\bar{\psi}\mathcal{D}\psi$ $J(\alpha)$: Jacobian under the chiral transformation
- Therefore, the action transforms as (Chiral) Anomaly!!!

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \ e^{iS[\bar{\psi},\psi,A_{\mu}]} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \ e^{iS[\bar{\psi},\psi,A_{\mu}] + \log J(\alpha)} = iS(\alpha)$$

Chiral Anomaly

• In (3+1)-d, the chiral anomaly can be computed as

$$S(\alpha) = -i \log J(\alpha) = -\frac{e^2}{16\pi^2} \int d^3x dt \ \alpha \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}.$$

- This method for computing anomalies is called
 Fujikawa's method.
 Fujikawa, Phys. Rev. Lett., (1979)
 Fujikawa, Phys. Rev. D, 21, (1980)
- Recently, there has been significant progress in the study of anomalies, but I cannot understand all the key concepts.

Derivation of Effective Action of 3D TIs

- By computing the chiral anomaly, we derive the effective action of 3D TIs.
- The effective Hamiltonian for 3D TIs Zhang, et al., Nat. Phys., (2009)

$$H(\mathbf{k}) = k_x \alpha^1 + k_y \alpha^2 + k_z \alpha^3 + m\alpha^4$$

Clifford algebra: $\{\alpha^a, \alpha^b\} = 2\delta^{ab}$ $m > 0 \rightarrow \text{Topological Insulators}$ $m < 0 \rightarrow \text{Trivial Insulators}$

• The action for 3D trivial insulators

$$S[\bar{\psi},\psi,A_{\mu}] = \int d^4x \ \bar{\psi}[i\gamma^{\mu}D_{\mu} + m]\psi, \ \gamma^i = \alpha^0 \alpha^i.$$

Derivation of Effective Action of 3D TIs

• On the other hand, the action for 3D TIs

$$S[\bar{\psi},\psi,A_{\mu}] = \int d^4x \ \bar{\psi}[i\gamma^{\mu}D_{\mu}] \psi, \ \gamma^i = \alpha^0 \alpha^i.$$

- These two action can be continuously $\psi \to \psi' = e^{-i\pi\gamma^5/2}\psi$ connected to the chiral transformation. $\bar{\psi} \to \bar{\psi}' = \bar{\psi}e^{-i\pi\gamma^5/2}$
- Therefore, the effective action from the chiral anomaly

$$S\left(-\frac{\pi}{2}\right) = S_{\theta} = \frac{e^2}{32\pi^2} \int d^3x dt \ \theta \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}, \ \theta = \pi$$

Axion term!!!

Dynamical Axion Fields

- \checkmark The Axion field of 3D TIs is quantized to $\pi.$
- ✓ If a system has either time reversal or spatial invarsion symmetry, the Axion field is quantized to 0 or π .
- Let us consider the following effective Hamiltonian

$$H(\mathbf{k}) = k_x \alpha^1 + k_y \alpha^2 + k_z \alpha^3 + m\alpha^4 + m'\alpha^5, \ \alpha^5 = \alpha^1 \alpha^2 \alpha^3 \alpha^4.$$

 $T^{-1}H(k)T \neq H(-k) \rightarrow No \text{ time reversal symmetry}$ $P^{-1}H(k)P \neq H(-k) \rightarrow No \text{ spatial inversion symmetry}$

Fujikawa's
$$\theta = \frac{\pi}{2}(1 + \operatorname{sgn}(m)) - \arctan \frac{m'}{m}$$
 Takes any values!!!

Dynamical Axion Fields

 In a lattice system, Antiferromagnetic 3D TIs can realize this Axion field with space-time dependence.

> <u>Sekine and Nomura, J. Phys. Soc. Jpn., (2014)</u> <u>Sekine and Nomura, Phys. Rev. Lett., (2016)</u>

 Remember the modified Maxwell equations

 $\left(\boldsymbol{j} = c \nabla \times \boldsymbol{M} + \frac{\partial \boldsymbol{P}}{\partial t} \right)$

$$\nabla \times \boldsymbol{H} - \frac{1}{c} \frac{\partial \boldsymbol{D}}{\partial t} = \frac{4\pi}{c} \boldsymbol{j}$$
$$\boldsymbol{D} = \boldsymbol{E} + 4\pi \boldsymbol{P} + \frac{\alpha}{\pi} \theta \boldsymbol{B} = \epsilon \boldsymbol{E} + \frac{\alpha}{\pi} \theta \boldsymbol{B}$$
$$\boldsymbol{H} = \boldsymbol{B} - 4\pi \boldsymbol{M} + \frac{\alpha}{\pi} \theta \boldsymbol{E} = \frac{\boldsymbol{B}}{\mu} + \frac{\alpha}{\pi} \theta \boldsymbol{E}$$

 $\checkmark P$ and M can be interpreted as an electric current.

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Dynamical Axion Fields

• An electric current originates from the Axion field

$$\boldsymbol{j} = \boldsymbol{j}_{\text{AHE}} + \boldsymbol{j}_{\text{CME}} = \frac{e^2}{2\pi h} \left[\nabla \theta(t, \boldsymbol{x}) \times \boldsymbol{E} + \frac{1}{c} \frac{\partial \theta(t, \boldsymbol{x})}{\partial t} \boldsymbol{B} \right]$$

$$\boldsymbol{j}_{\mathrm{AHE}} = rac{e^2}{2\pi h} \nabla \theta(t, \boldsymbol{x}) \times \boldsymbol{E}$$
: Anomolus Hall Effect
 $\boldsymbol{j}_{\mathrm{CME}} = rac{e^2}{2\pi h} rac{1}{c} rac{\partial \theta(t, \boldsymbol{x})}{\partial t} \boldsymbol{B}$: Chiral Magnetic Effect

• Surface half quantized hall currents correspond to $j_{
m AHE}$.

Weyl Semimetals

• Weyl semimetals as an example of dynamical Axion fields

$$H(\boldsymbol{k}) = \boldsymbol{k} \cdot \left(\tau^3 \otimes \boldsymbol{\sigma}\right) + \boldsymbol{b} \cdot \left(I \otimes \boldsymbol{\sigma}\right) - \mu_5 \left(\tau^3 \otimes I\right)$$

The action for Weyl semimetals

$$S = \int d^4x \; \bar{\psi} i \gamma^{\mu} \big[\partial_{\mu} - i e A_{\mu} - i b_{\mu} \gamma^5 \big] \psi$$

$$b_{\mu} = (\mu_5, -b)$$
: Chiral gauge field

2b
$2\mu_5$

Weyl Semimetals

• By applying Fujikawa's method, <u>Zyuzin and Burkov, Phys. Rev. B, (2012)</u> <u>Vazifeh and Franz, Phys. Rev. Lett., (2013)</u>

$$S_{\theta} = \frac{e^2}{32\pi^2} \int d^3x dt \ \theta(t, \boldsymbol{x}) \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}, \ \theta(t, \boldsymbol{x}) = -2b_{\mu} x^{\mu}$$

Computing the electric current, we obtain

$$oldsymbol{j}_{ ext{AHE}} = rac{e^2}{\pi h}oldsymbol{b} imes oldsymbol{E}, \ oldsymbol{j}_{ ext{CME}} = -rac{e^2}{\pi h}\mu_5oldsymbol{B}$$

• In equilibrium states, the chiral magnetic effect cannot be realized.

Vazifeh and Franz, Phys. Rev. Lett., (2013)

20

 $12\mu_5$

Conclusion

- The topological field theory that describes topological responses in 3D TIs can be obtained via dimensional reduction from the (4+1)-d Chern-Simons gauge theory.
- Topological electromagnetic responses in 3D TIs originate from a single Dirac cone at the surface.
- There are some topological materials where Axion emerge.