

# 反強磁性絶縁体アキシオン

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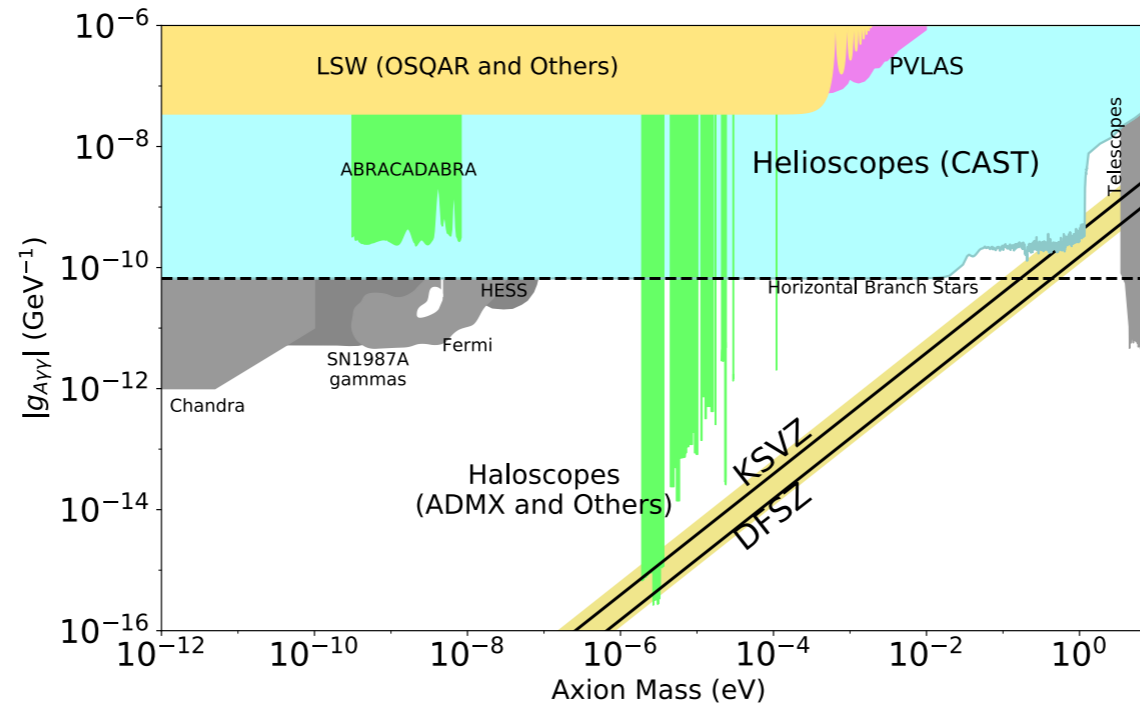
# **1. Introduction**

## Axion and axion-like particles (ALPs)

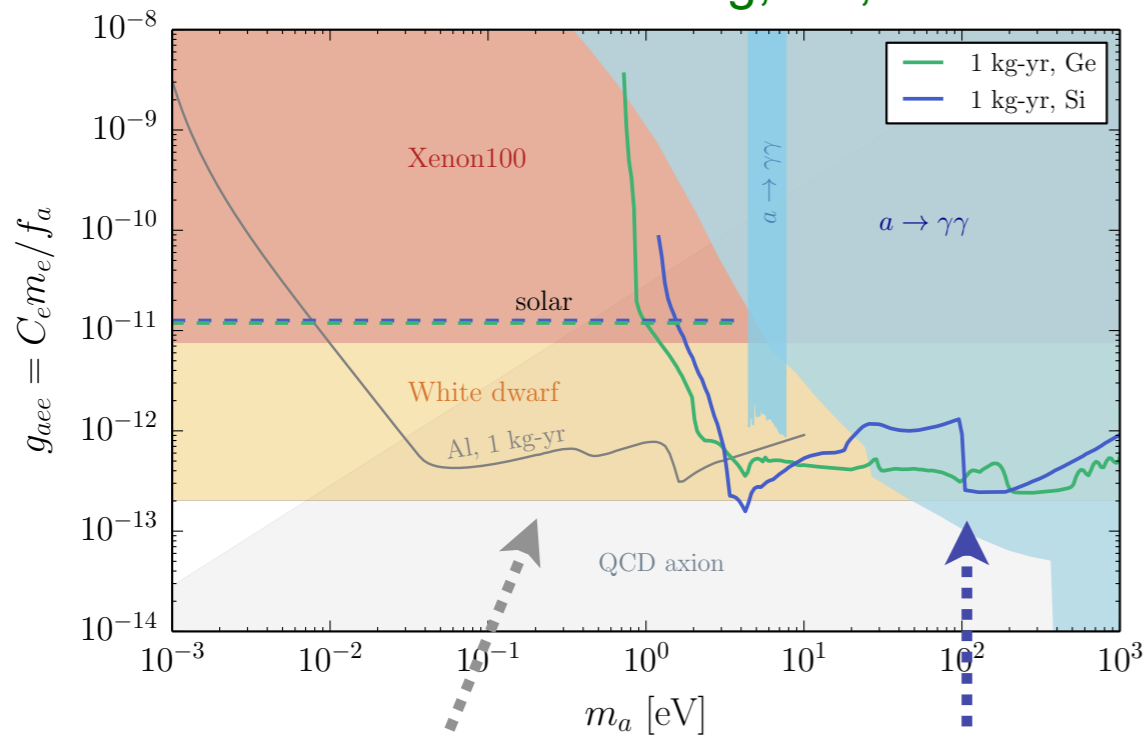
- A solution to the strong CP problem (for axion)
- DM candidates
- Inspired by superstring theory
- Impacts on cosmology (axion strings, domain walls, mini-clusters, etc.)

# Axion and ALPs search

PDG '20



Hochberg, Lin, Zurek '17

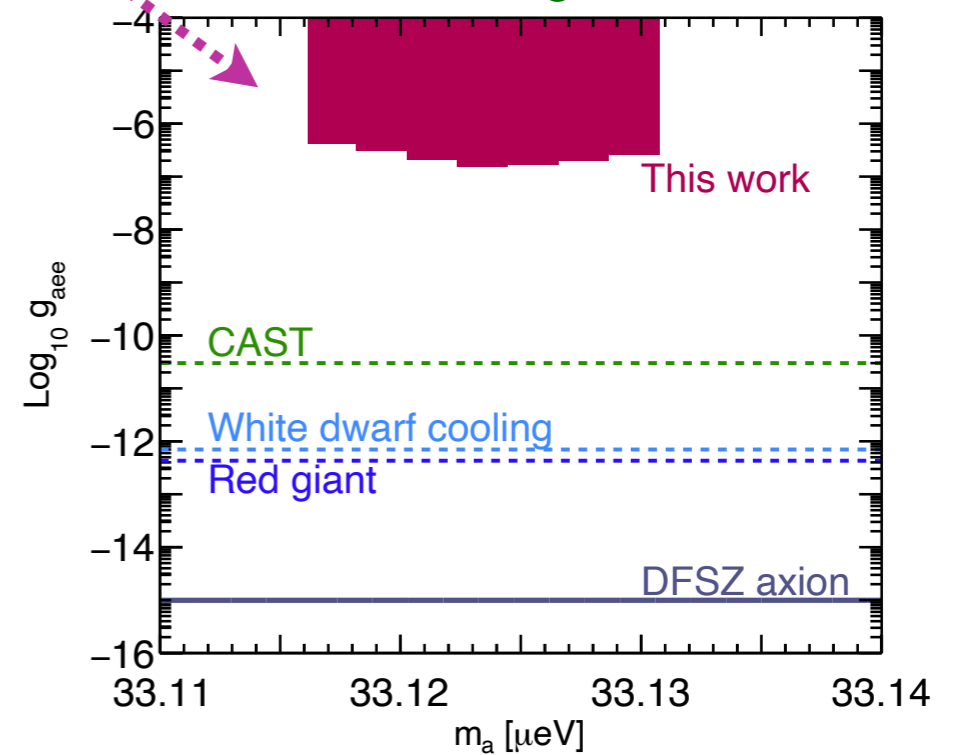


superconductors

semiconductors

magnon

Ikeda, Ito, Miuchi, Soda, Kurashige, Shikano '21



## Axion and axion-like particles (ALPs)

- A solution to the strong CP problem (for axion)
- DM candidates
- Inspired by superstring theory
- Impacts on cosmology (axion strings, domain walls, mini-clusters, etc.)
- Lots of searching using various techniques are ongoing

## Axion and axion-like particles (ALPs)

- A solution to the strong CP problem (for axion)
- DM candidates
- Inspired by superstring theory
- Impacts on cosmology (axion strings, domain walls, mini-clusters, etc.)
- Lots of searching using various techniques are ongoing
- 'Axion' is predicted in topological insulators
- 'Axion' in insulators can be used for axion detection

# Axion is predicted in topological magnetic insulators

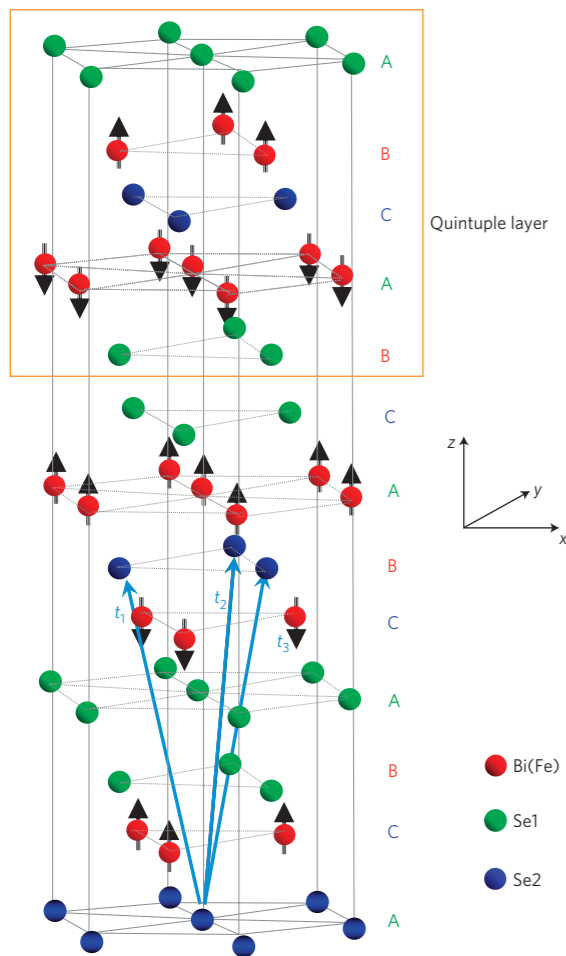
ARTICLES

PUBLISHED ONLINE: 7 MARCH 2010 | DOI: 10.1038/NPHYS1534

nature  
physics

## Dynamical axion field in topological magnetic insulators

Rundong Li<sup>1</sup>, Jing Wang<sup>1,2</sup>, Xiao-Liang Qi<sup>1</sup> and Shou-Cheng Zhang<sup>1\*</sup>



Bi<sub>2</sub>Se<sub>3</sub>

(Topological insulator)

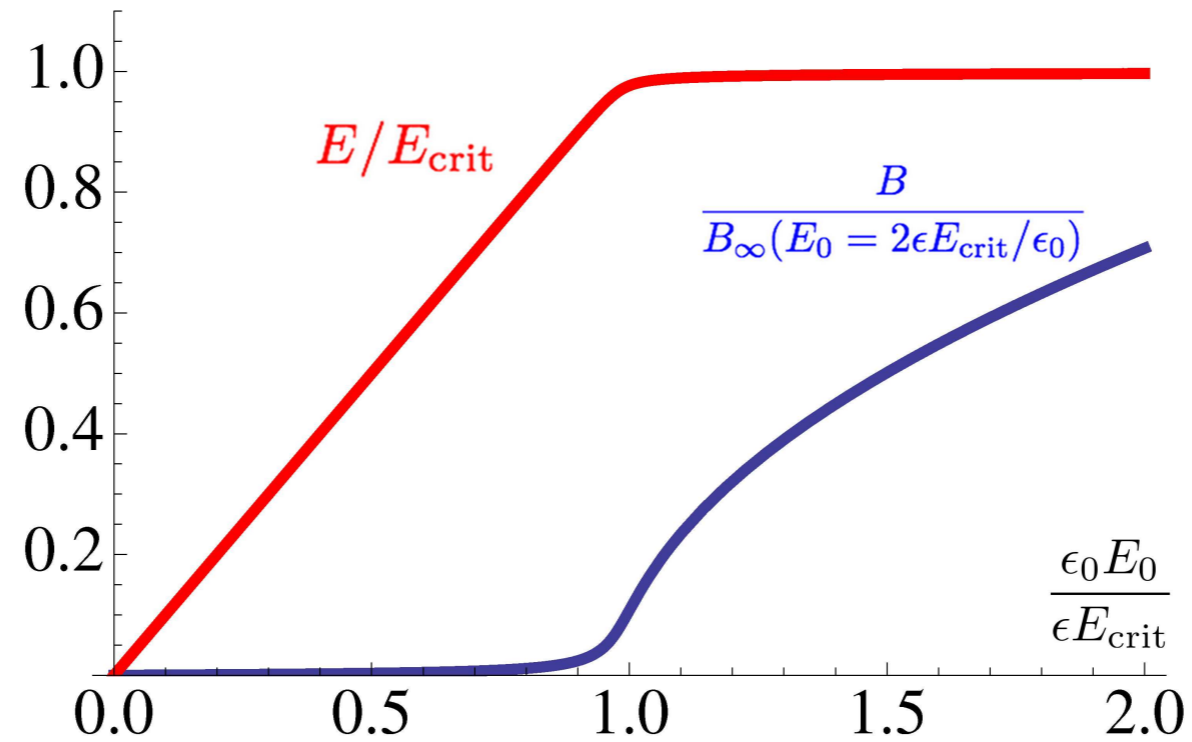
$$\begin{aligned}
 \mathcal{S}_{\text{tot}} &= \mathcal{S}_{\text{Maxwell}} + \mathcal{S}_{\text{topo}} + \mathcal{S}_{\text{axion}} \\
 &= \frac{1}{8\pi} \int d^3x dt \left( \epsilon \mathbf{E}^2 - \frac{1}{\mu} \mathbf{B}^2 \right) + \frac{\alpha}{4\pi^2} \int d^3x dt (\theta_0 + \delta\theta) \mathbf{E} \cdot \mathbf{B} \\
 &\quad + g^2 J \int d^3x dt [(\partial_t \delta\theta)^2 - (v_i \partial_i \delta\theta)^2 - m^2 \delta\theta^2] \quad (4)
 \end{aligned}$$

$\theta F_{\mu\nu} \tilde{F}^{\mu\nu}$

Axion mass  $\sim \mathcal{O}(\text{meV})$

# Axion induces instability in insulators

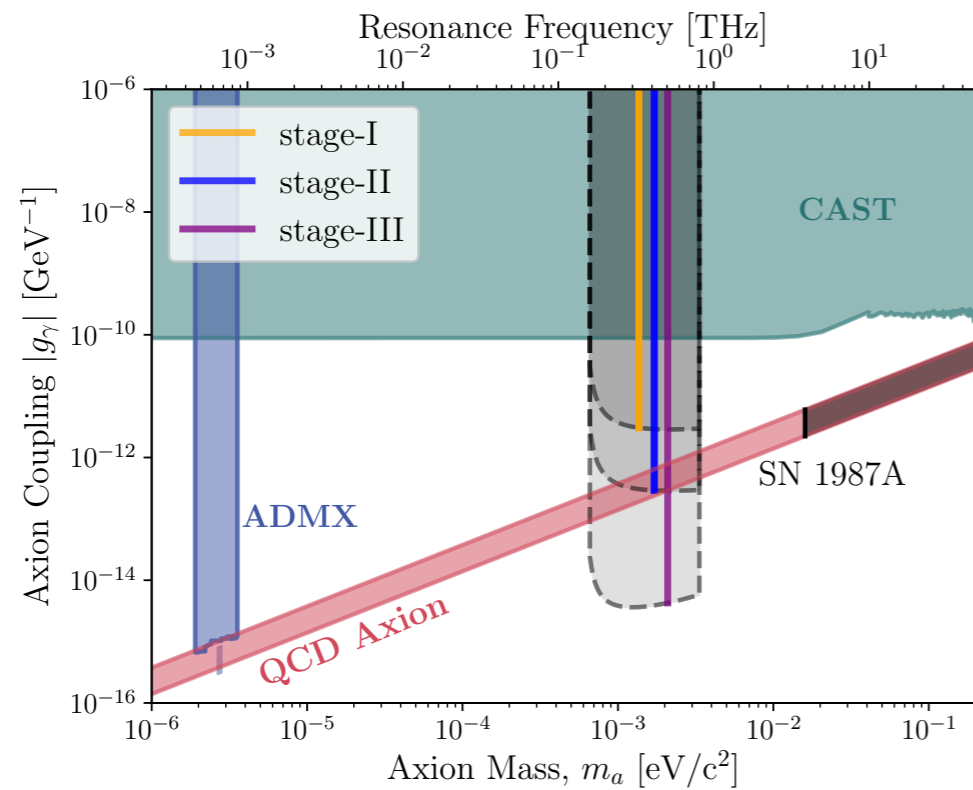
Ooguri, Oshikawa '12



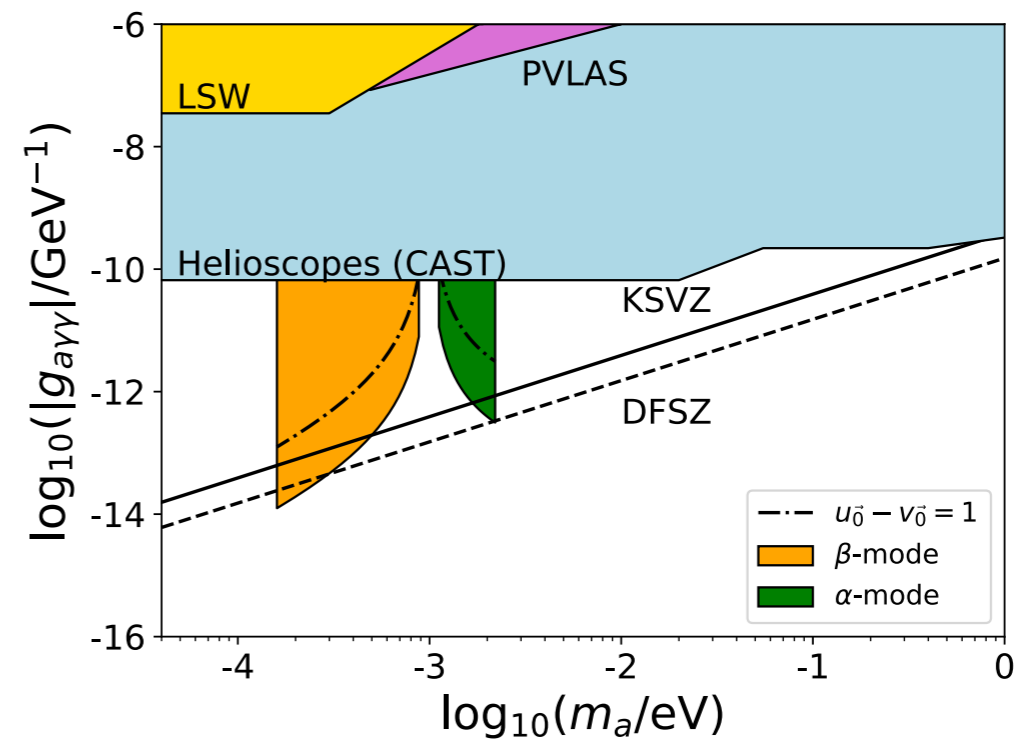
Axion-photon coupling  $\longrightarrow$  Instability of photon  
 $\longrightarrow$  Magnetic field is induced



# Proposals for axion/ALPs search using 'axion' in insulators



Marsh, Fong, Lentz, Smejkal, Ali '19



Chigusa, Moroi, Nakayama '21

Keywords: topological insulator, magnetism

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Today, I would like to address

- What is topological insulator?
- How does magnetism play a role?
- How is 'axion' in insulators described?

## Plan to talk

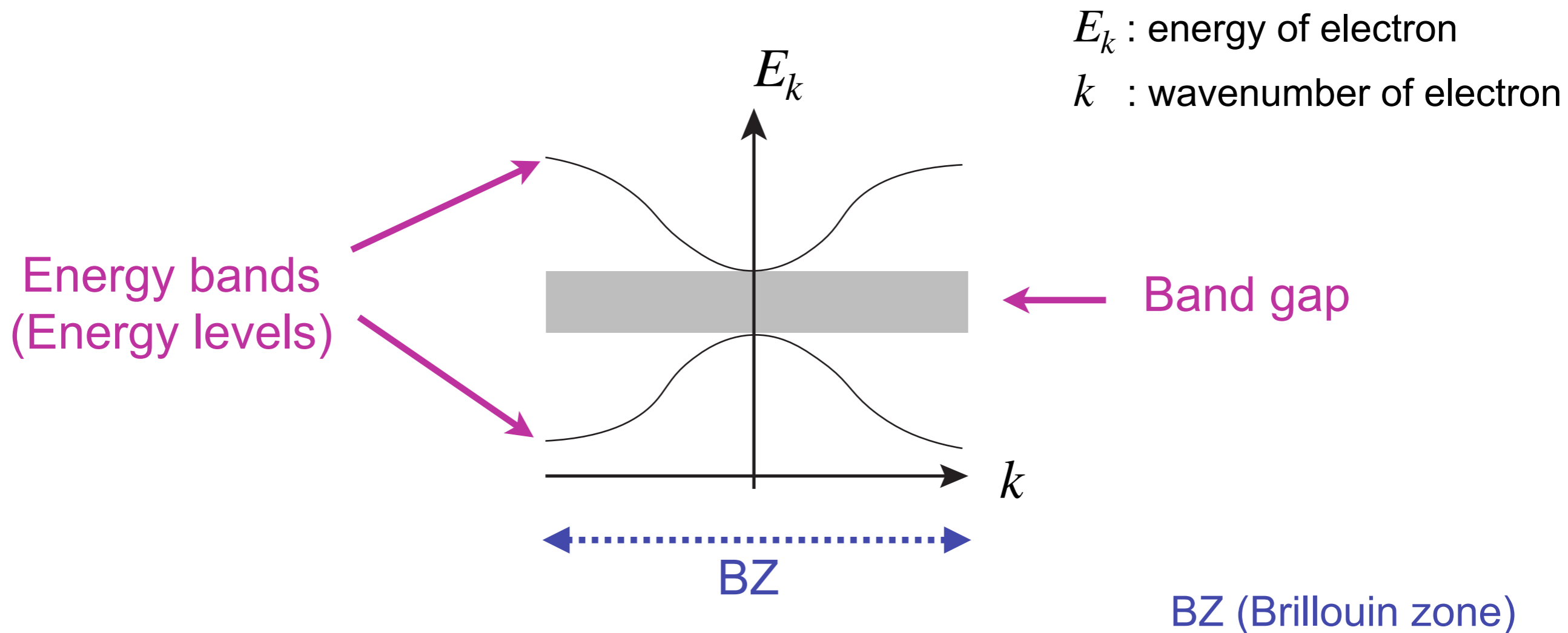
1. Introduction
2. Brief review of condensed matter physics (related to axion)
3. Axion in antiferromagnetic topological insulators
4. Conclusions and discussion

## **2. Brief review of condensed matter physics (related to axion)**

## Topics related to axion in condensed matter physics

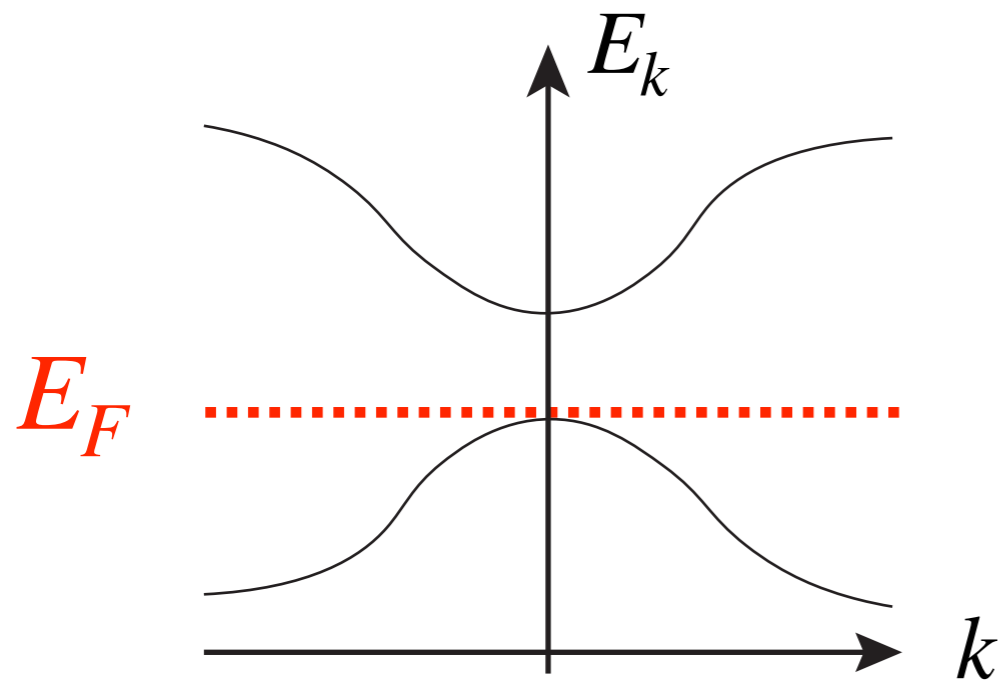
- a). Insulators
- b). Anomalous quantum Hall effect
- c). Topological insulators
- d). Magnetoelectric effect

## Minimum basics



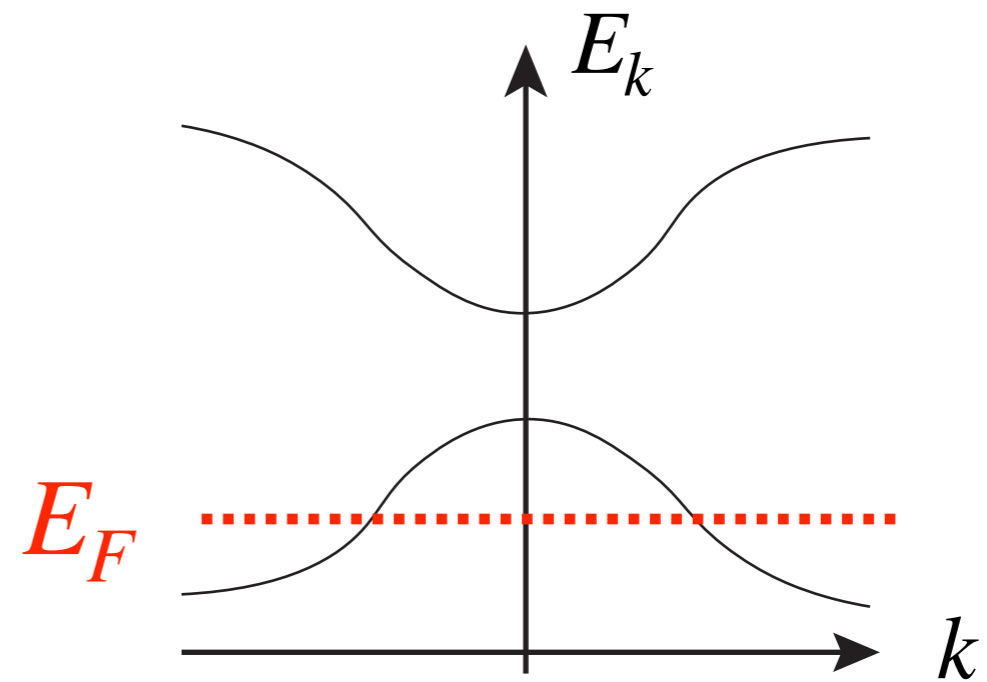
The region where there is no energy level is called **band gap** (important for insulators)

Insulator



Fermi energy is in the band gap

Metal



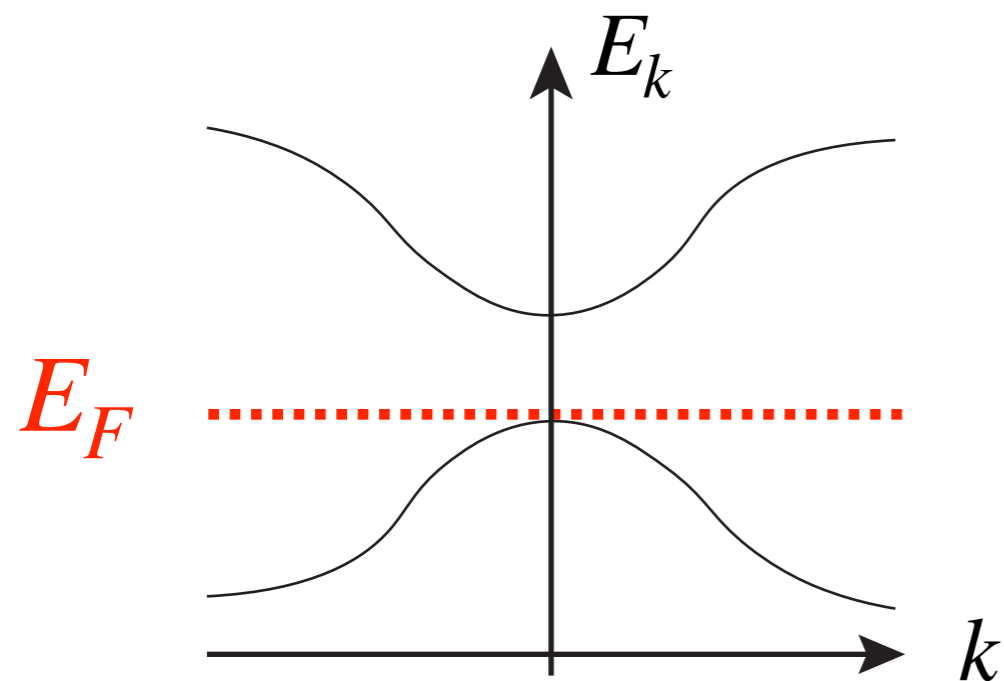
Fermi energy is in the band

$E_F$  : Fermi energy

Fermi energy are important to distinguish  
insulators and metals

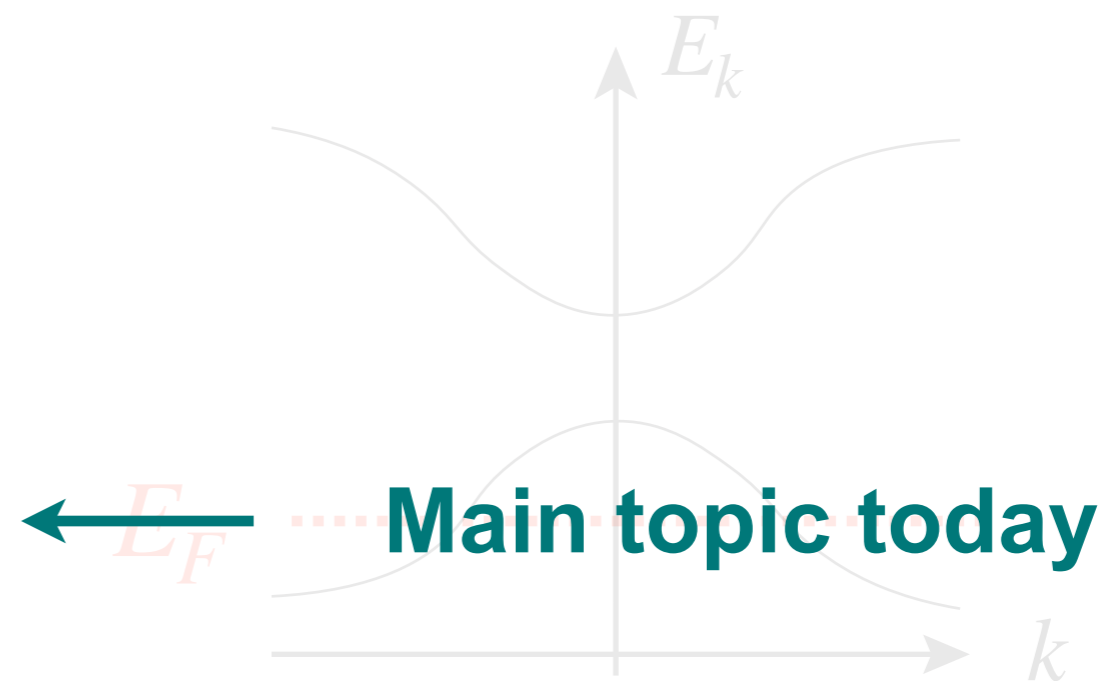


### Insulator



Fermi energy is in the band gap

### Metal



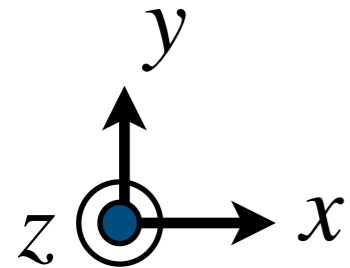
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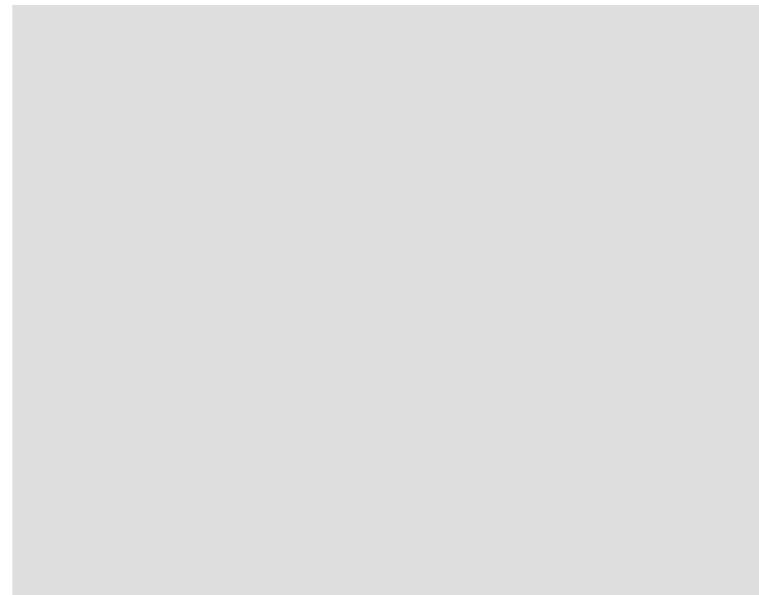
Fermi energy are important to distinguish insulators and metals

# Quantum Hall (QH) effect

e.g., 2D insulator



⊙  $B$  : magnetic field



↑  $E$  : electric field

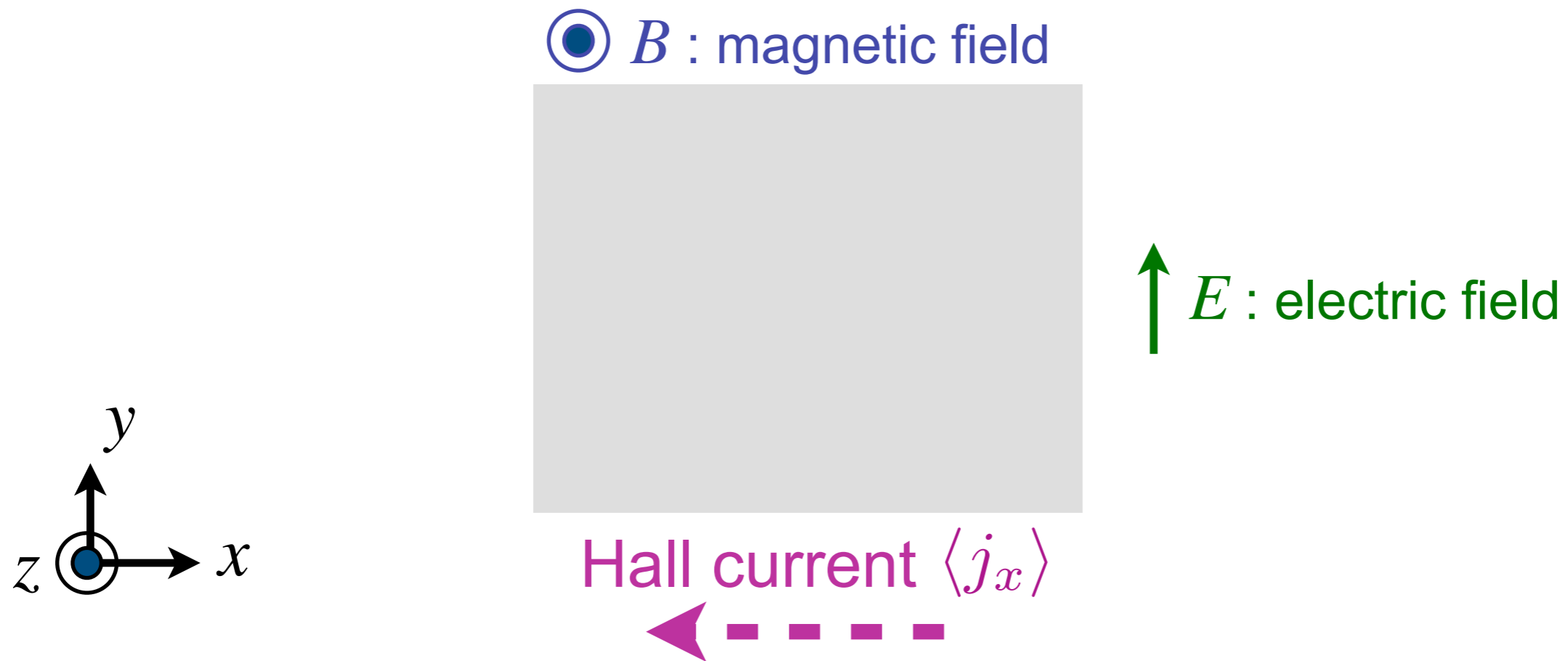
b). Anomalous quantum Hall effect

QH effect appears in semiconductor too

Quantum Hall (QH) effect

e.g., 2D insulator

QH effect appears in semiconductor too



*Quantized* electric current is induced in  $x$  direction

## b). Anomalous quantum Hall effect

Thouless, Kohmoto, Nightingale, den Nijs '82

It seems weird but there was theoretical prediction:

Hall conductivity:

$$\begin{aligned}\sigma_{xy} &\equiv \langle j_x \rangle / E_y \\ &= \nu \frac{e^2}{h}\end{aligned}$$

*TKNN formula*

$$\begin{aligned}\nu &\equiv \sum_n \int_{\text{BZ}} \frac{d^2 k}{2\pi} [\nabla_{\mathbf{k}} \times \mathbf{a}_n(\mathbf{k})]_z \\ \mathbf{a}_n(\mathbf{k}) &\equiv -i \langle u_{n\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | u_{n\mathbf{k}} \rangle\end{aligned}$$

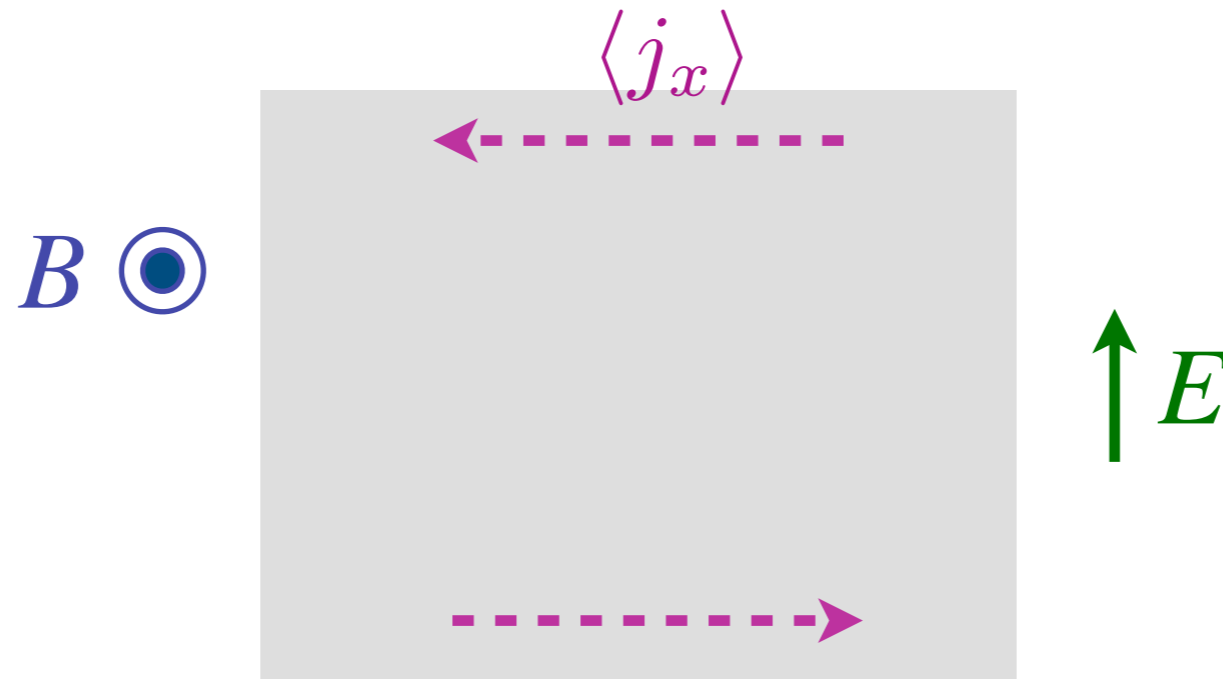
$|u_{n\mathbf{k}}\rangle$  : Bloch state

$n$  : label of band

→  $\nu$  is given by (half-) integer

“(Integer) QH effect”

The current flows at the edge



e.g., a toy model in 2D

$$H = \begin{pmatrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{pmatrix} = \mathbf{d} \cdot \boldsymbol{\sigma}$$

$$\mathbf{d} = (m, k_x, k_y)$$

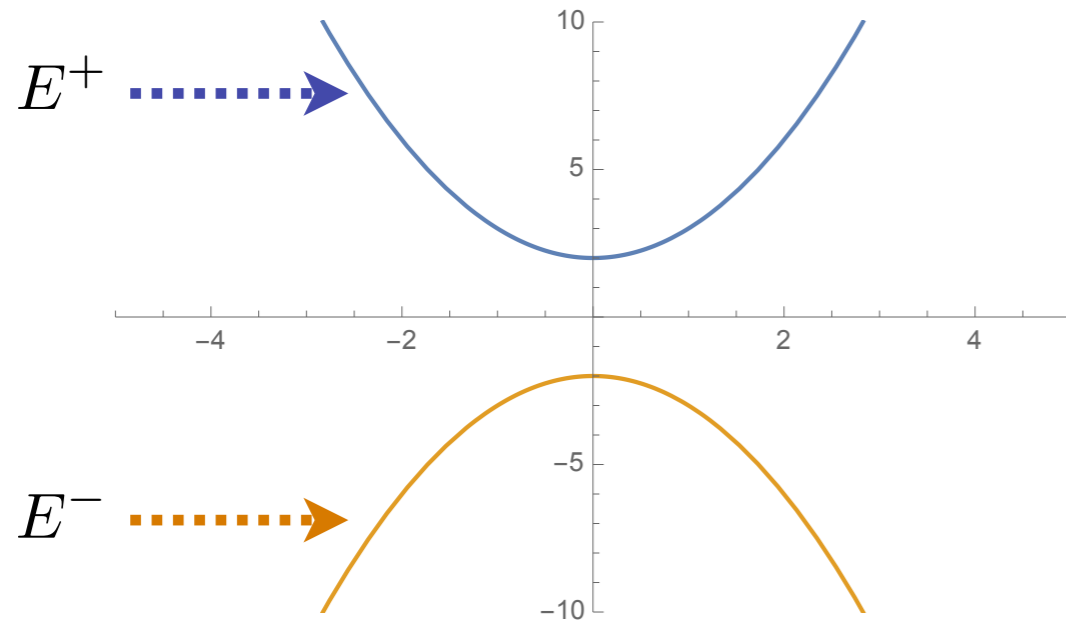


$$\begin{aligned} E^+ &\simeq m + \frac{|\mathbf{k}|^2}{2|m|} \\ E^- &\simeq -m - \frac{|\mathbf{k}|^2}{2|m|} \end{aligned}$$

around  $\mathbf{k} = 0$

The band structure

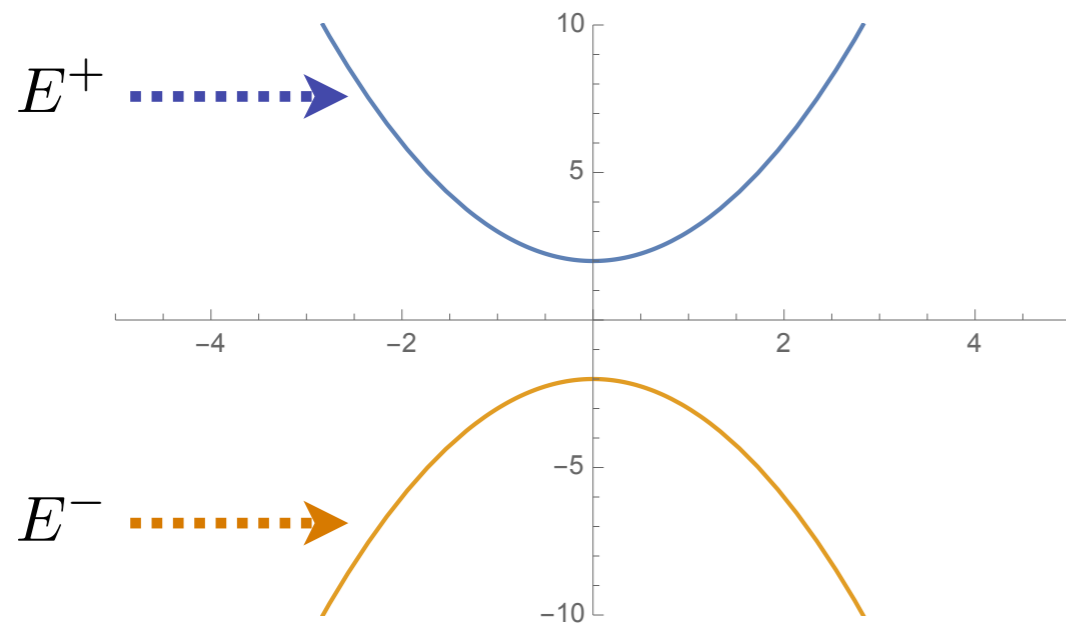
$$m > 0$$



Normal insulator

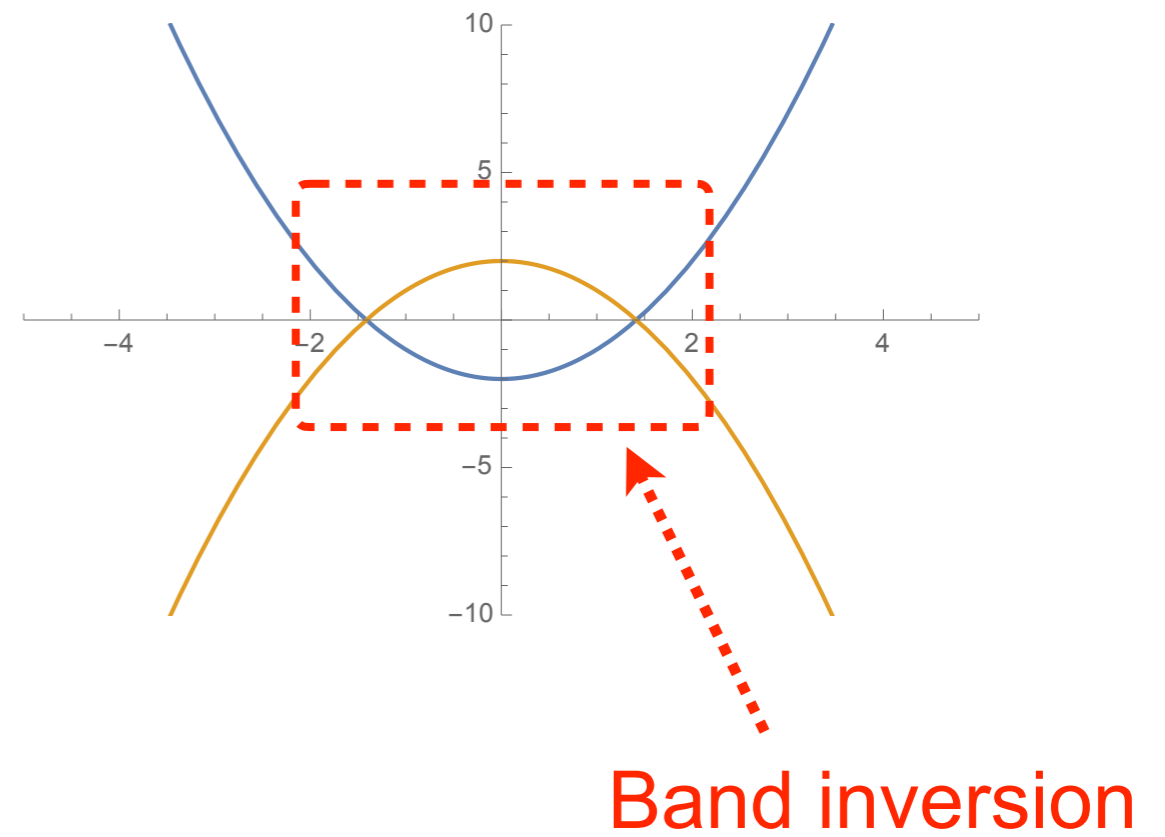
The band structure

$m > 0$



Normal insulator

$m < 0$



QH insulator

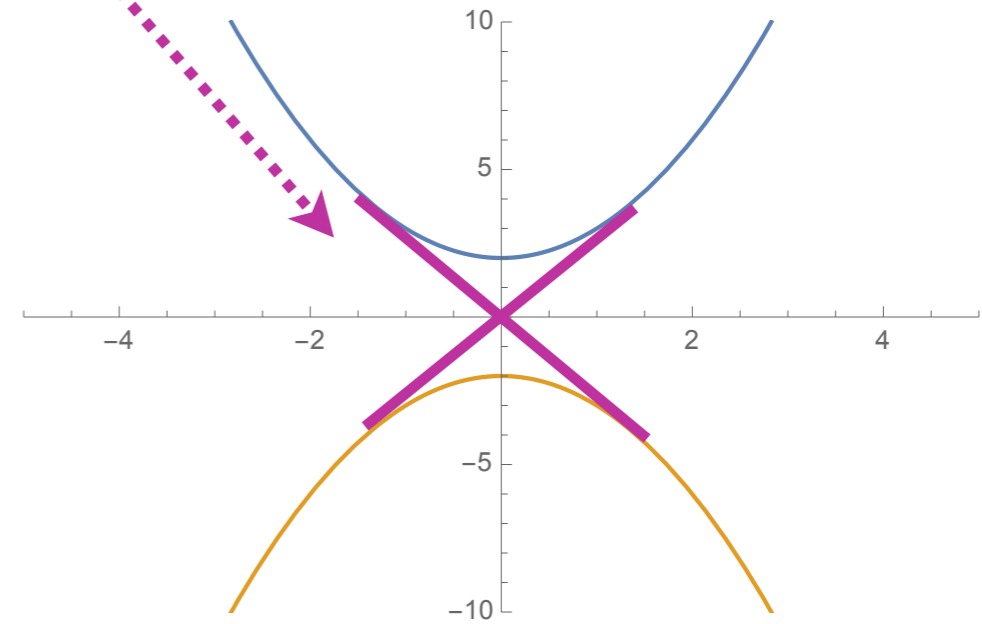
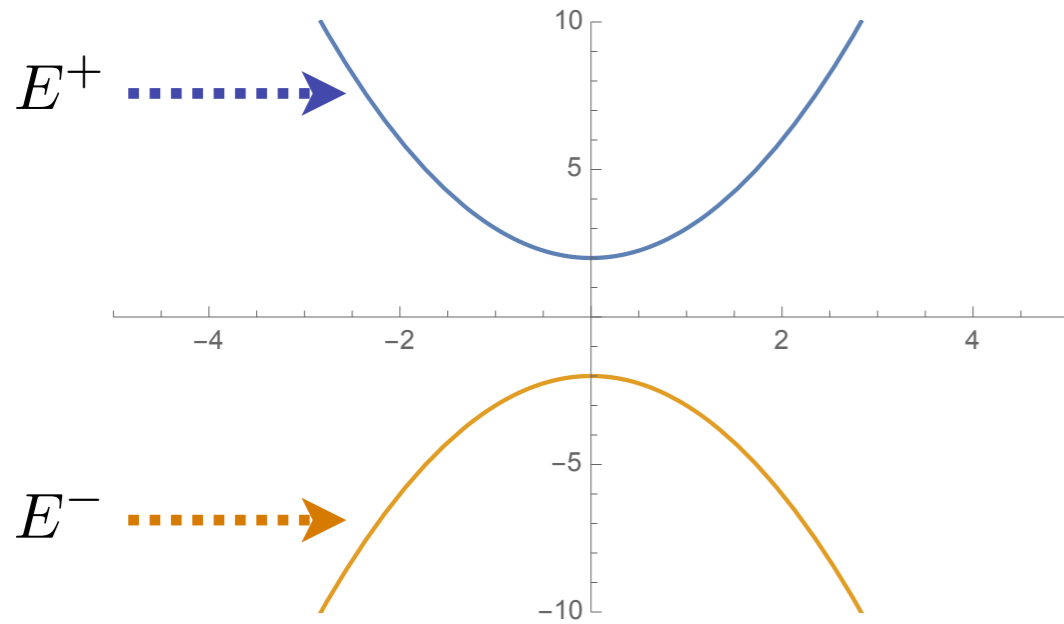


The band structure

Gapless states at edge

$m > 0$

$m < 0$

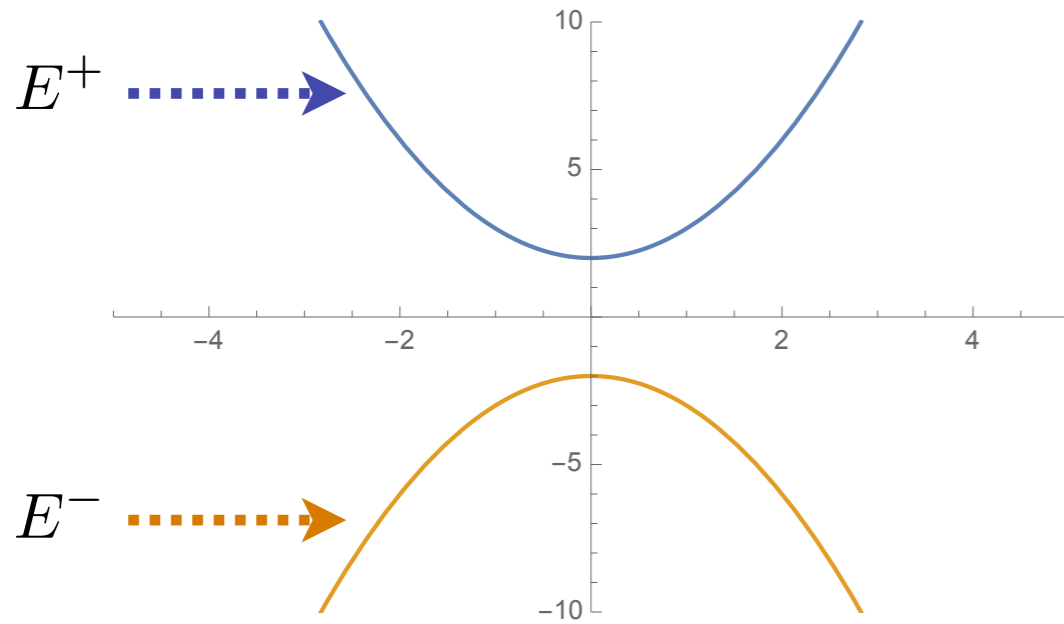


Normal insulator

QH insulator

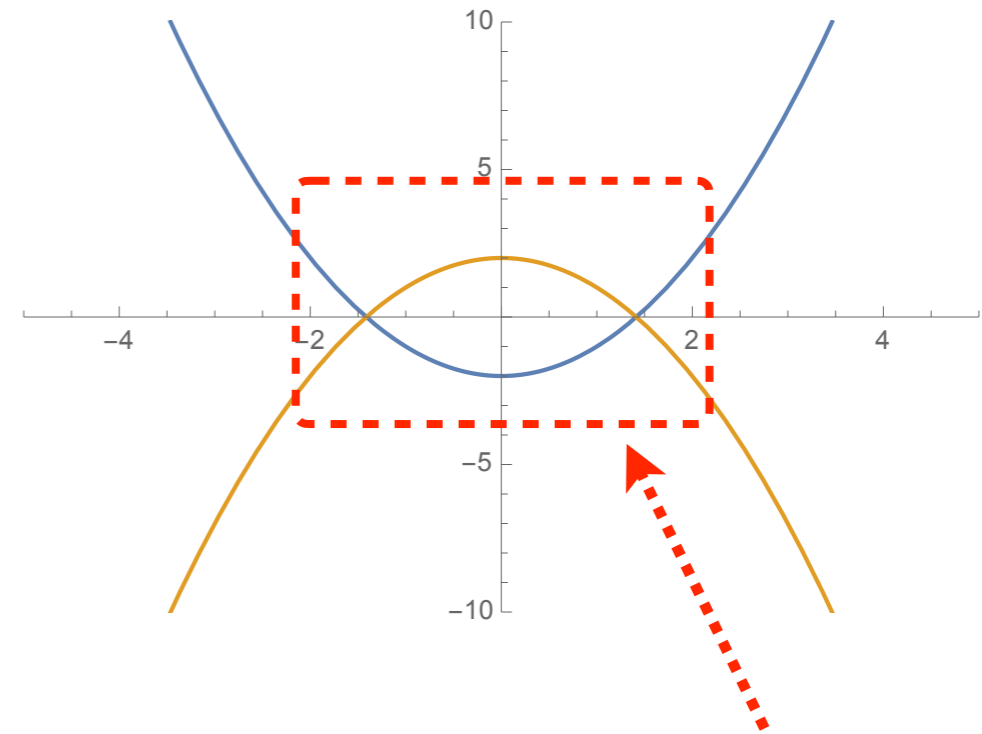
The band structure

$m > 0$



Normal insulator

$m < 0$



Band inversion

QH insulator

**Band inversion is important**

## Anomalous quantum Hall (AQH) effect

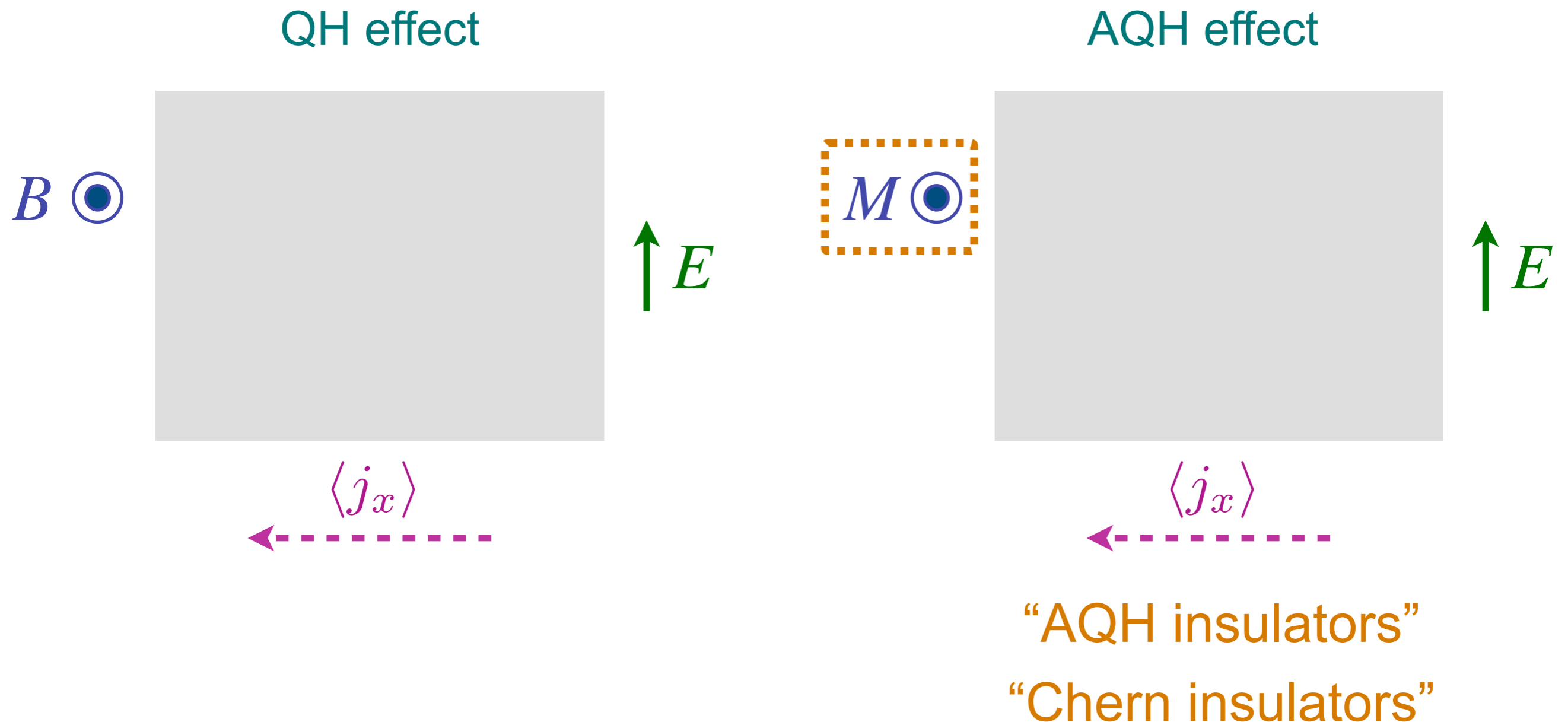
The same effect by magnetization  $M$ , not magnetic field

→ *Anomalous QH effect*

## Anomalous quantum Hall (AQH) effect

The same effect by magnetization  $M$ , not magnetic field

→ Anomalous QH effect



## Topics related to axion in condensed matter physics

a). Insulators

b). Anomalous quantum Hall effect

c). Topological insulators

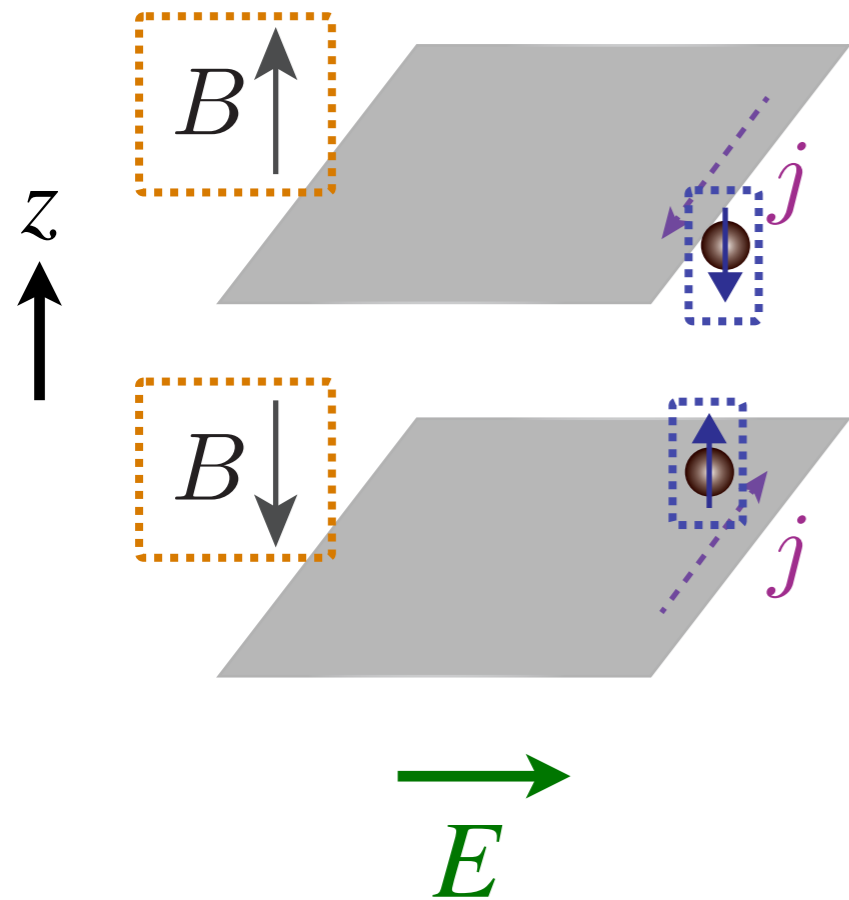
d). Magnetoelectric effect

# Topological insulators (TIs)

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Kane, Mele '05

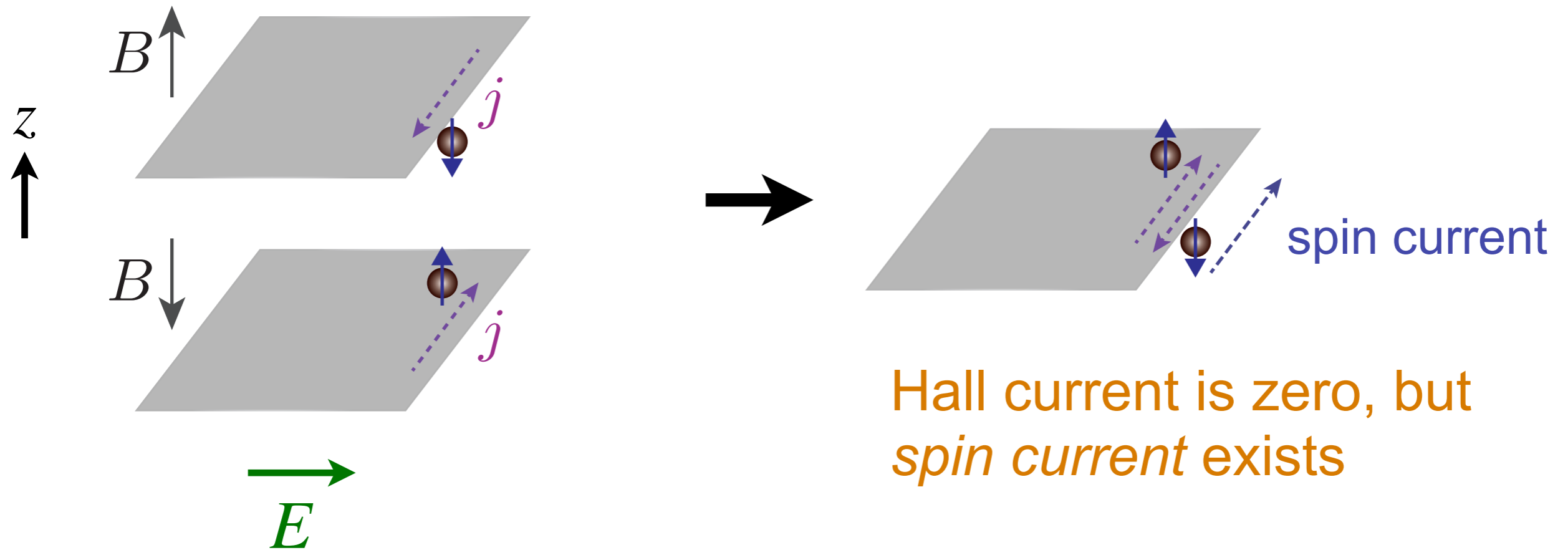
Idea: combination of two QH insulators



# Topological insulators (TIs)

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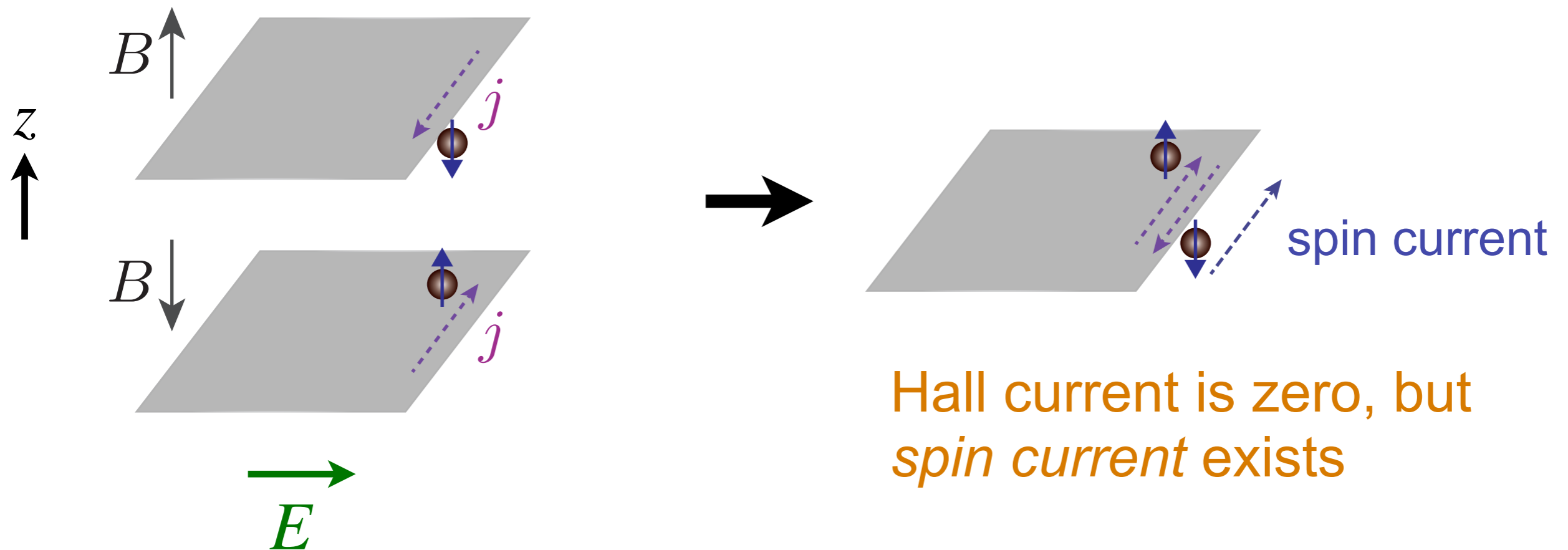




# Topological insulators (TIs)

Kane, Mele '05

Idea: combination of two QH insulators



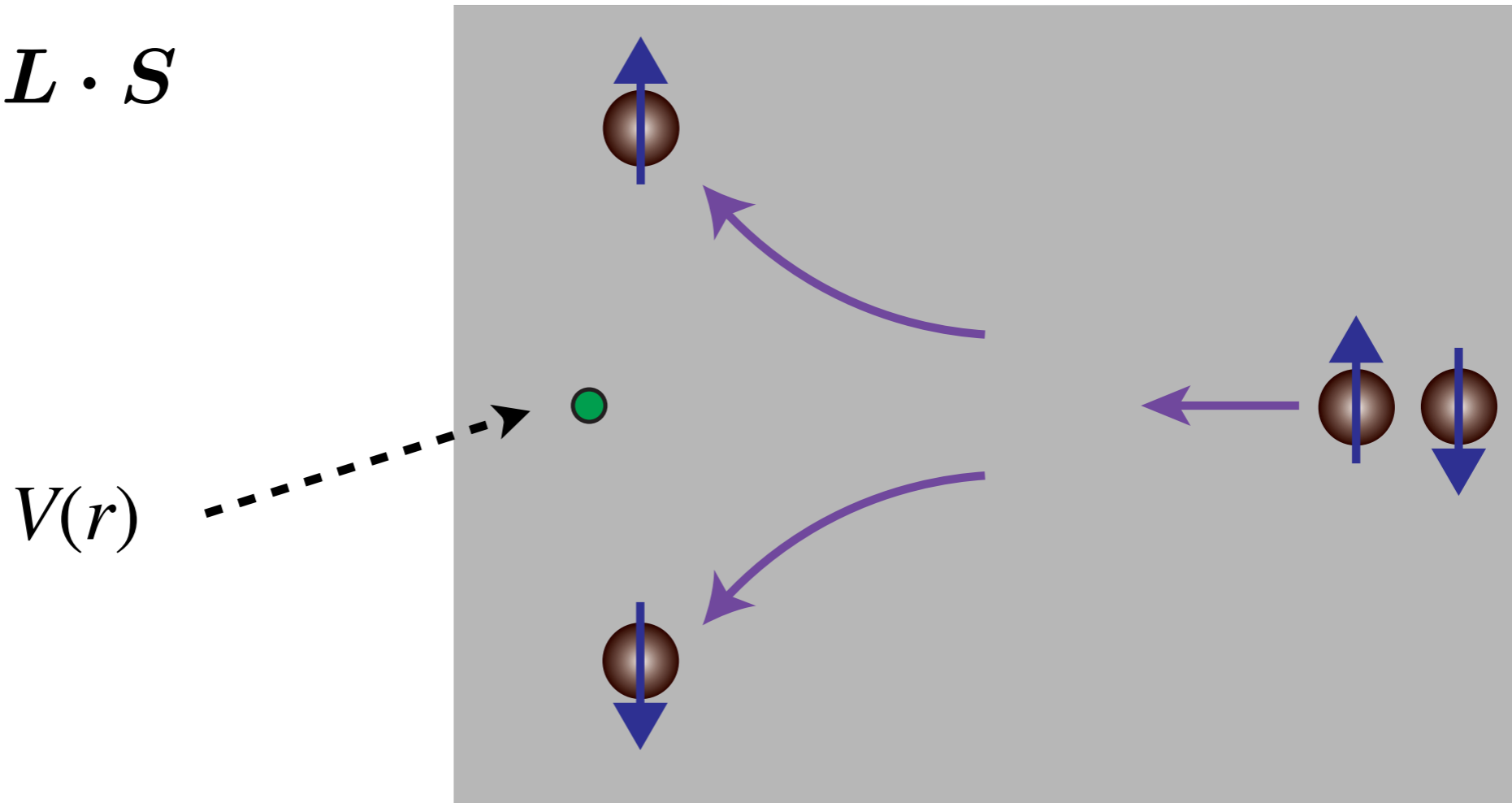
Such a system can be realized due to SOC  
(without magnetic field)

SOC: spin orbit coupling

## Spin-orbit coupling (SOC)

e.g.,

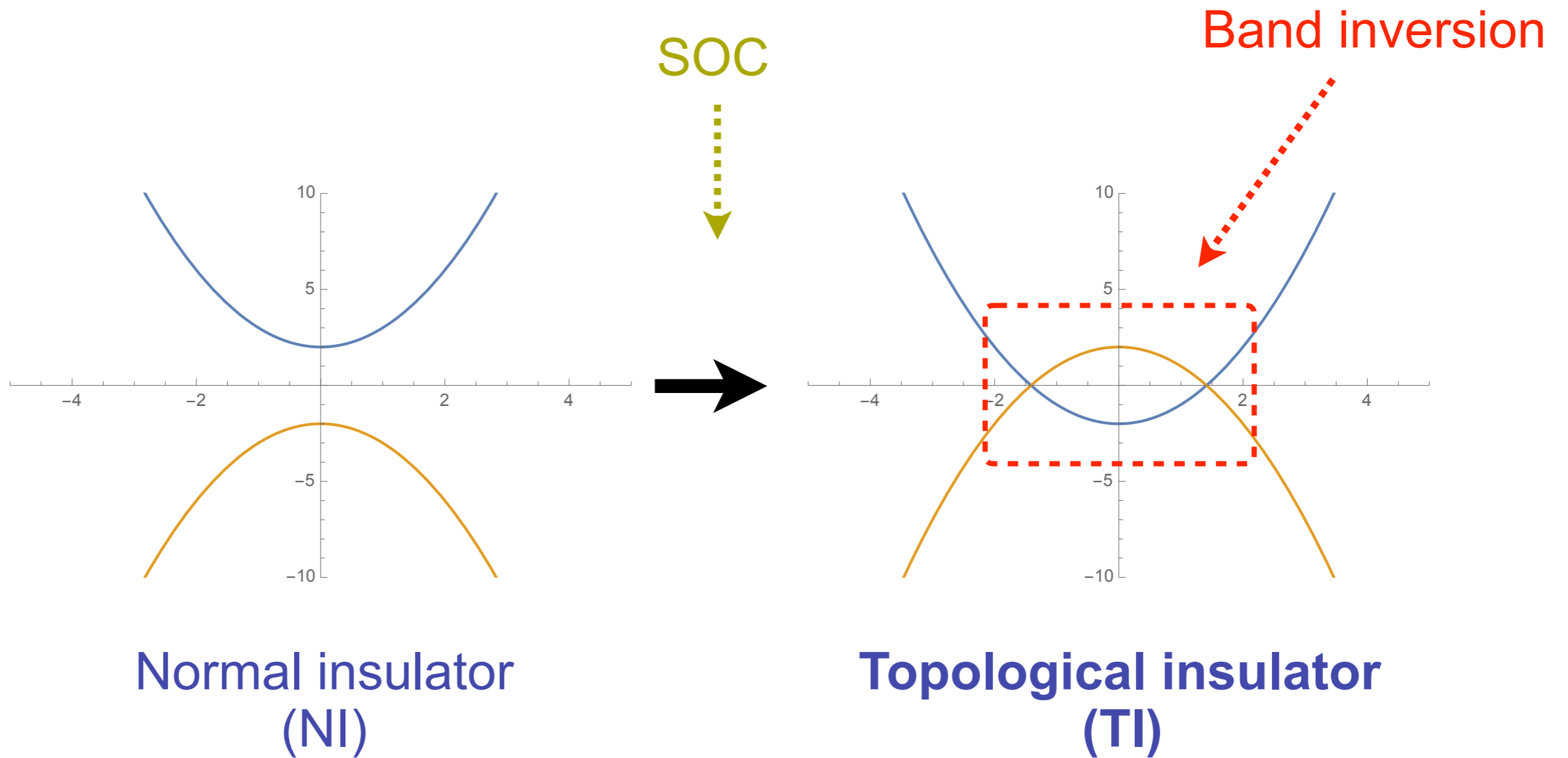
$$H_{\text{SO}} = V(r) \mathbf{L} \cdot \mathbf{S}$$



Electrons with spin up or down are scattered off to the opposite directions

# The band structure

→ The same as (A)QH insulators

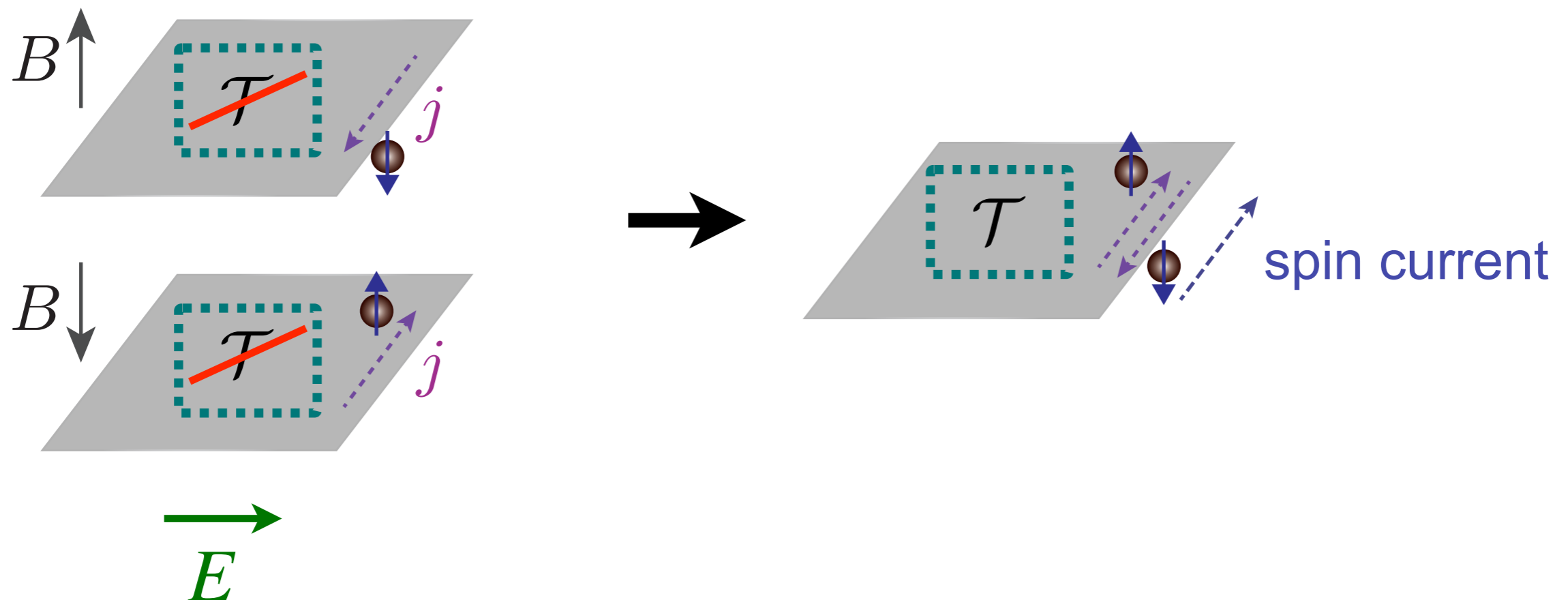


## Keywords for topological insulators

- Time reversal invariance ( $\mathcal{T}$ )
- Strong spin-orbit coupling (SOC)

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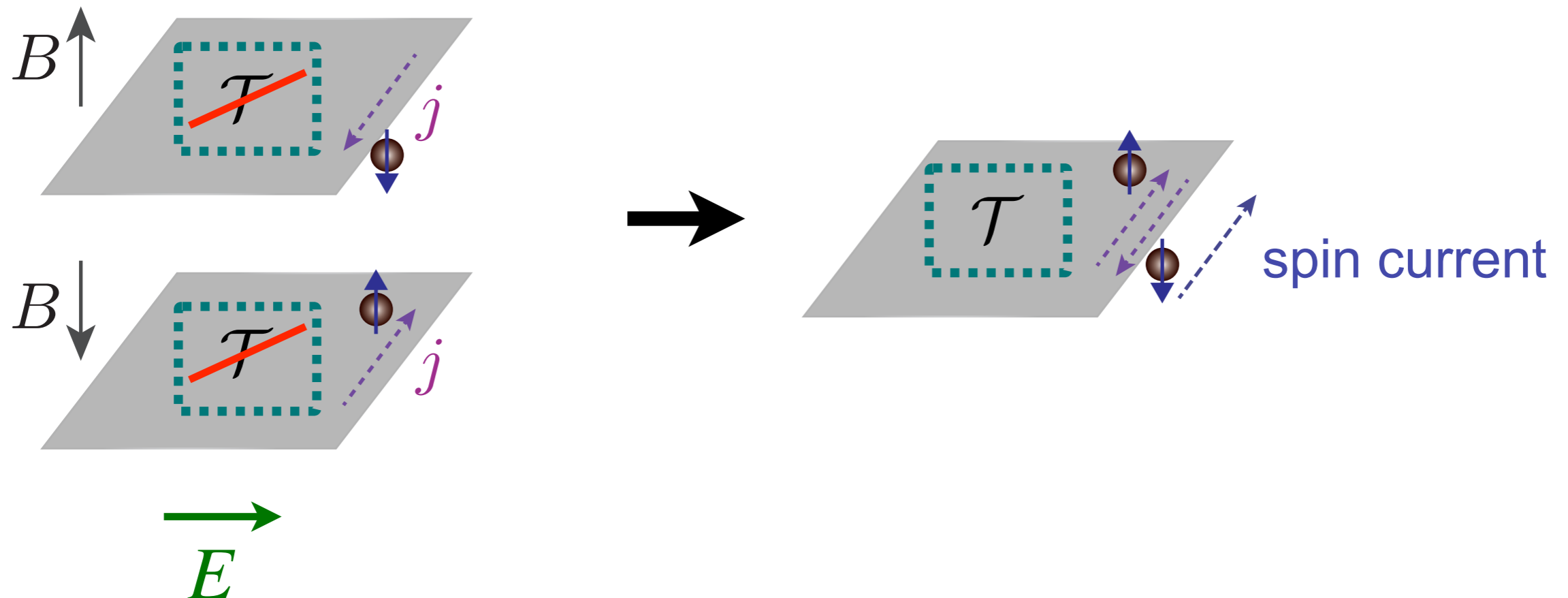
- Time reversal invariance ( $\mathcal{T}$ )
- Strong spin-orbit coupling (SOC)



$B$  breaks  $\mathcal{T}$  but the combination of  $B$  and  $-B$  keeps  $\mathcal{T}$

## Keywords for topological insulators

- Time reversal invariance ( $\mathcal{T}$ )
- Strong spin-orbit coupling (SOC)



Strong SOC is crucial for the realization

Magnetolectric (ME) effect

predicted by Landau&Lifshitz

discovered by Dzyaloshinskii '60

- Electric field ( $E$ ) induces magnetization  $M$
- Magnetic field ( $B$ ) induces electric polarization  $P$

$$M_j = \alpha_{ij} E_i$$

$$P_i = \alpha_{ij} B_j$$



$$F = -\frac{1}{\mu_0 c} \int d^3x \alpha_{ij} E_i B_j$$

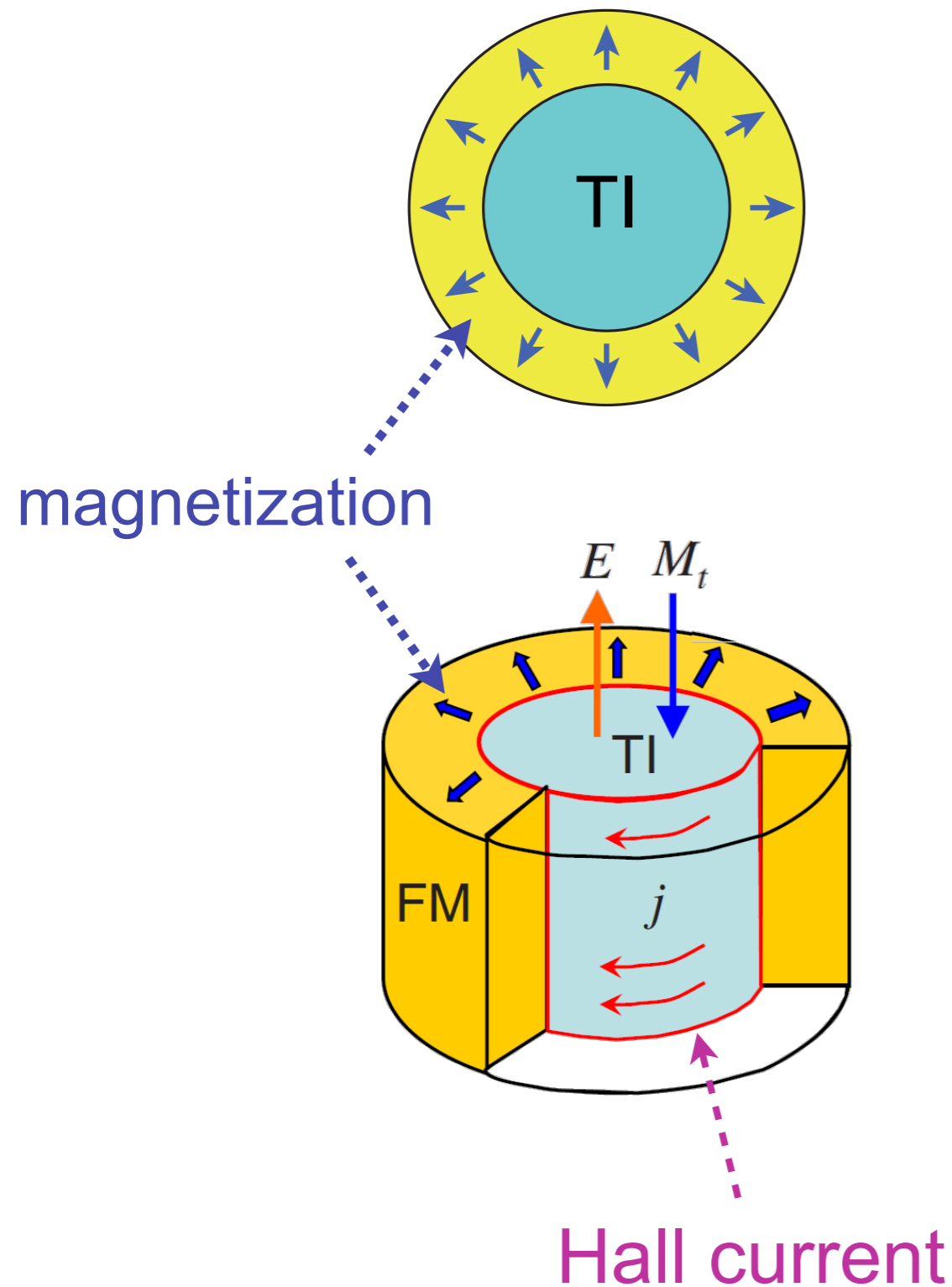
$$M_i = -\frac{1}{V} \left. \frac{\partial F}{\partial E_i} \right|_{B=0}$$

$$P_i = -\frac{1}{V} \left. \frac{\partial F}{\partial B_i} \right|_{E=0}$$

$\alpha_{ij}$  : constant

# 3D TI cylinder coated with magnetization directing outside

Qi, Hughes, Zhang '08



Half-integer AQH current



The current induces magnetization  
in  $z$  direction

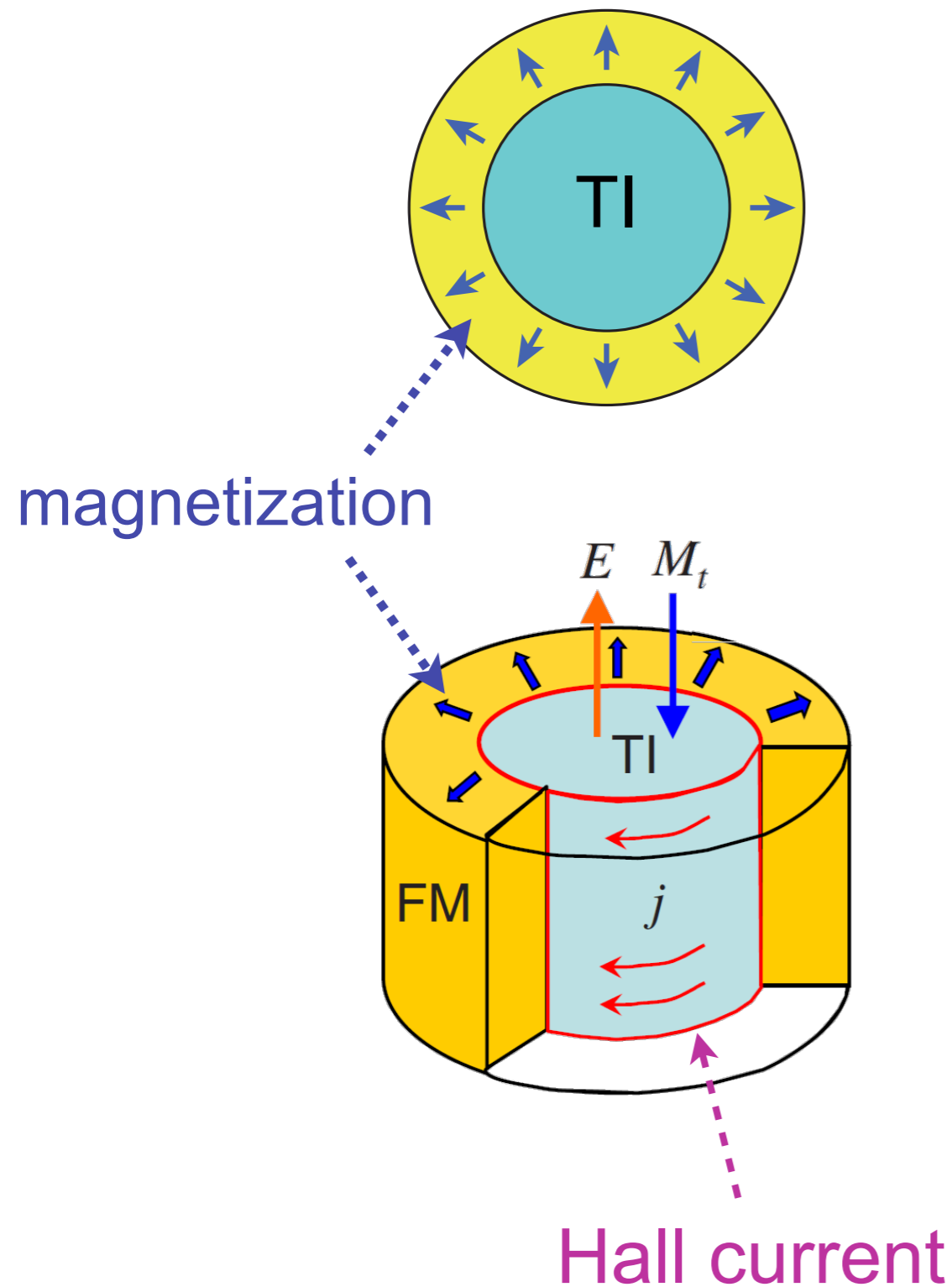
$$\mathbf{M} = \pm \frac{\alpha}{\mu_0 c} \mathbf{E}$$

$\alpha$  : fine-structure constant



# 3D TI cylinder coated with magnetization directing outside

Qi, Hughes, Zhang '08



Half-integer AQH current



The current induces magnetization  
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$$\mathbf{M} = \pm \frac{\alpha}{\mu_0 c} \mathbf{E}$$

The coefficient is given by  
fine-structure constant

$\alpha$  : fine-structure constant

This ME effect can be understood from the following free energy:

$$F_{\theta} = -\frac{1}{\mu_0} \int d^3x \frac{\alpha}{c\pi} \theta \mathbf{E} \cdot \mathbf{B} \quad \text{with} \quad \theta = \pm\pi$$

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$$\longrightarrow -\frac{\alpha}{4\pi} \theta F_{\mu\nu} \tilde{F}^{\mu\nu}$$

$\theta = \pm\pi$  is called static axion  
(  $\theta = 0$  in NI )

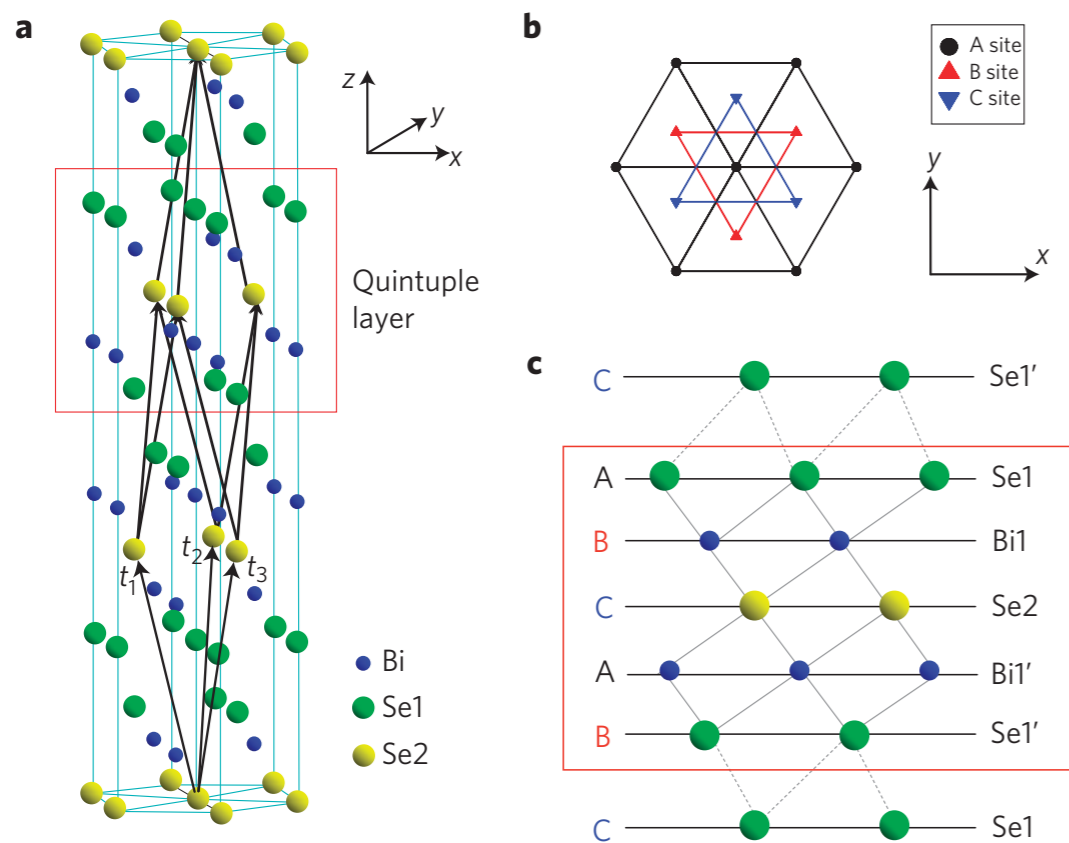
## Quick summary

- Fermi energy is in the band gap for insulators
- SOC and  $\mathcal{T}$  are crucial for TI
- ME effect in TI is described by “static axion”

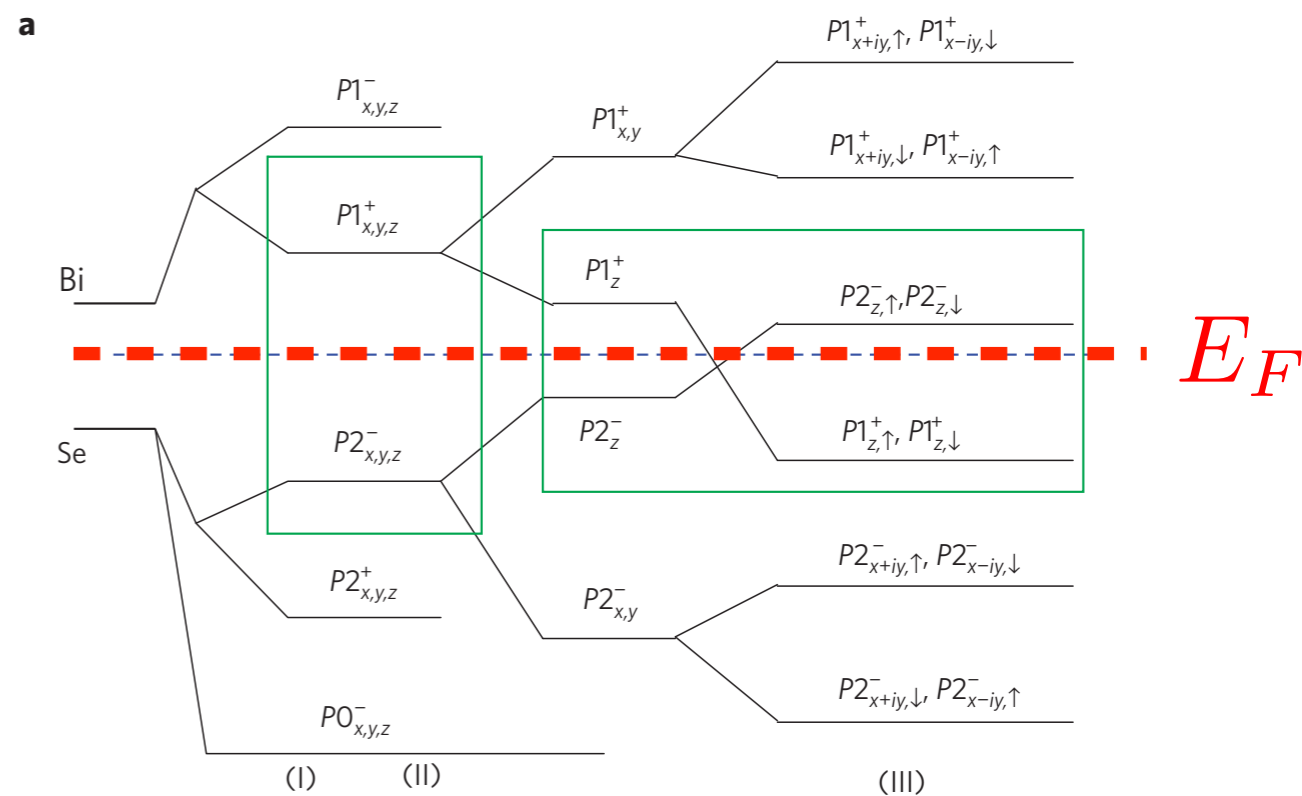
### **3. Axion in antiferromagnetic topological insulators**

# Let's consider 3D TI, $\text{Bi}_2\text{Se}_3$

H. Zhang et al. '09



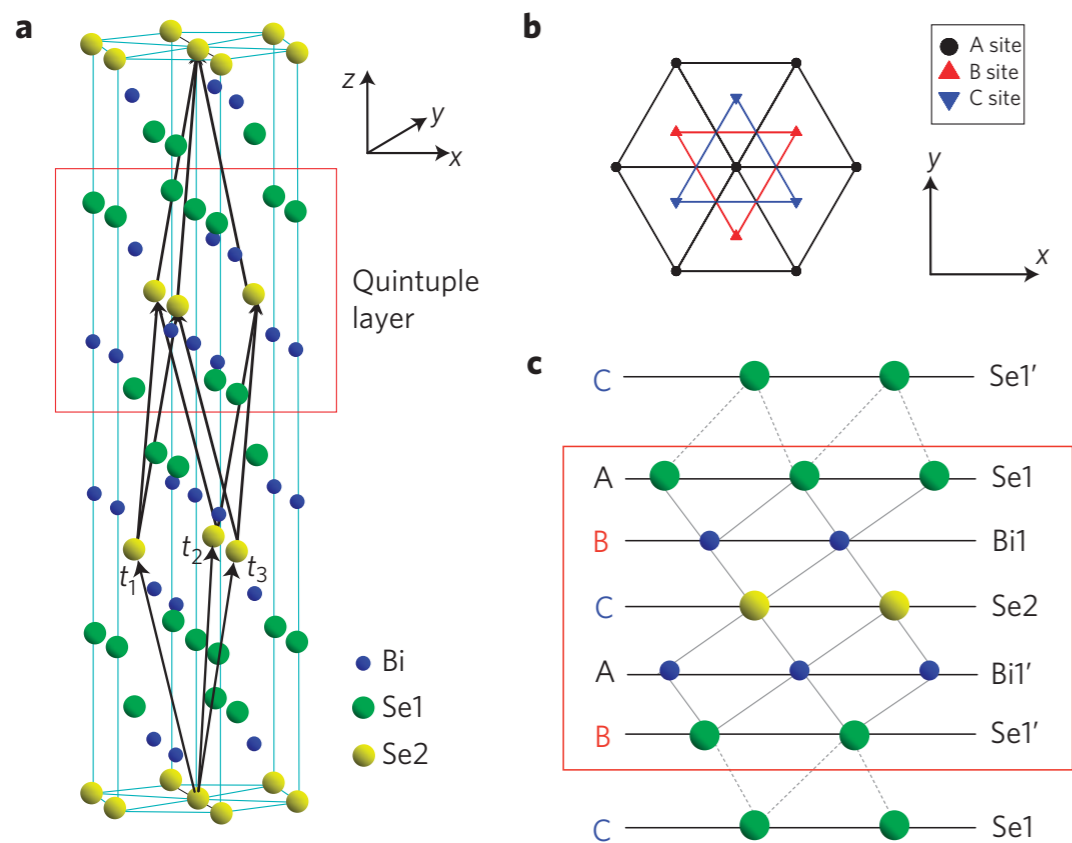
Crystal structure



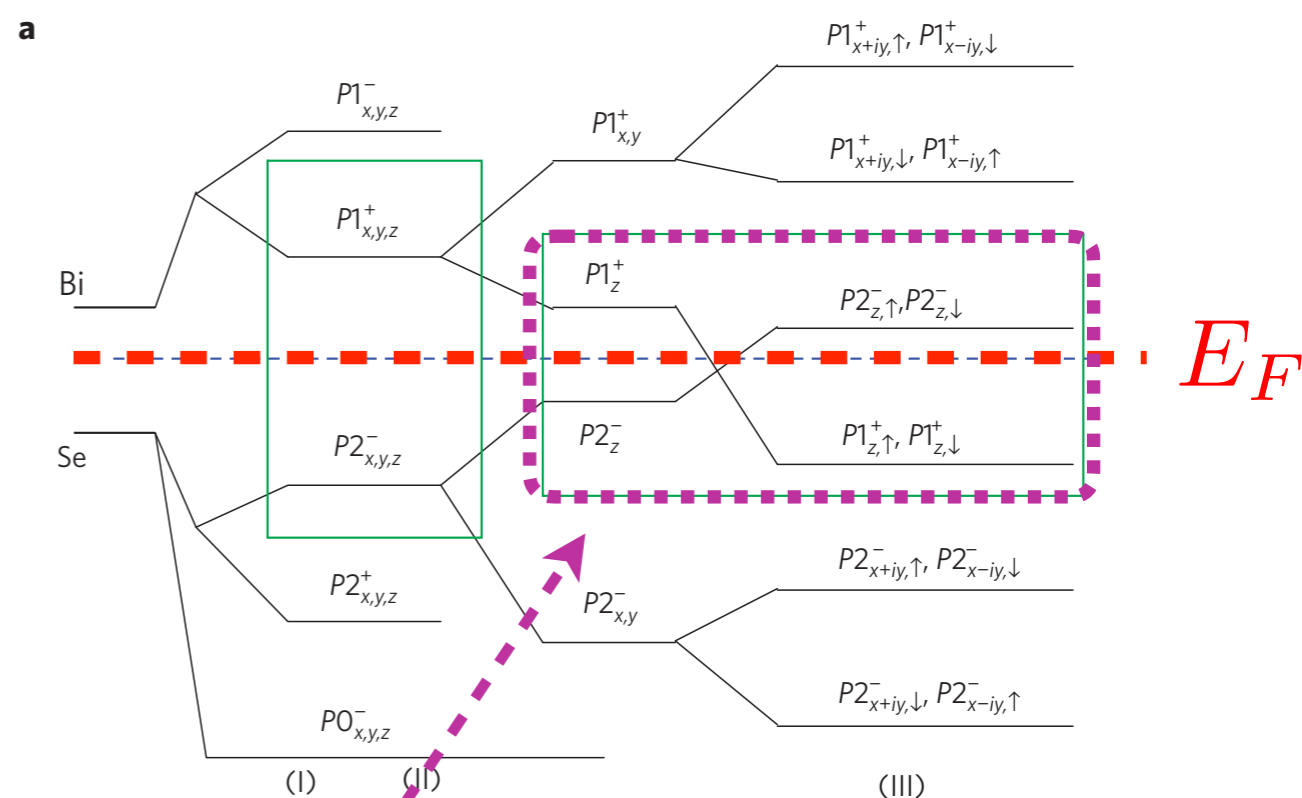
Energy levels

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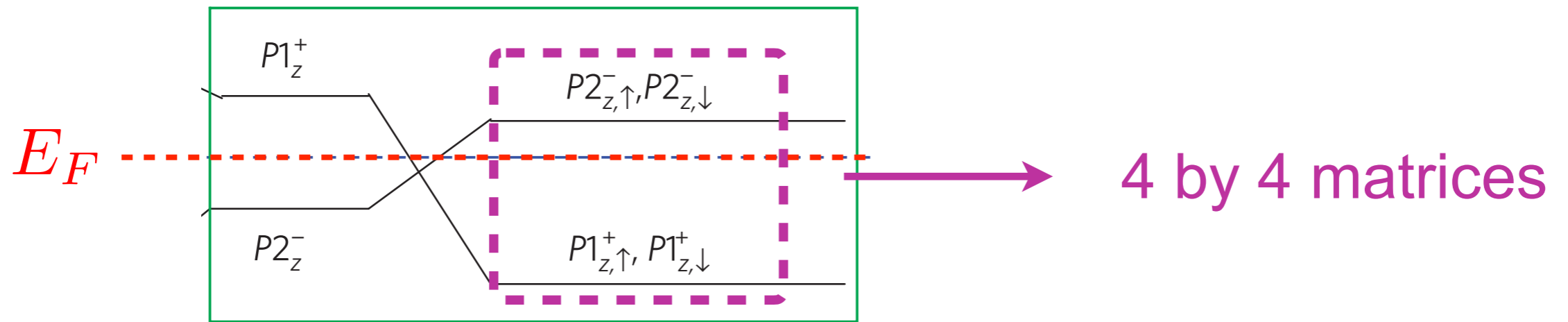
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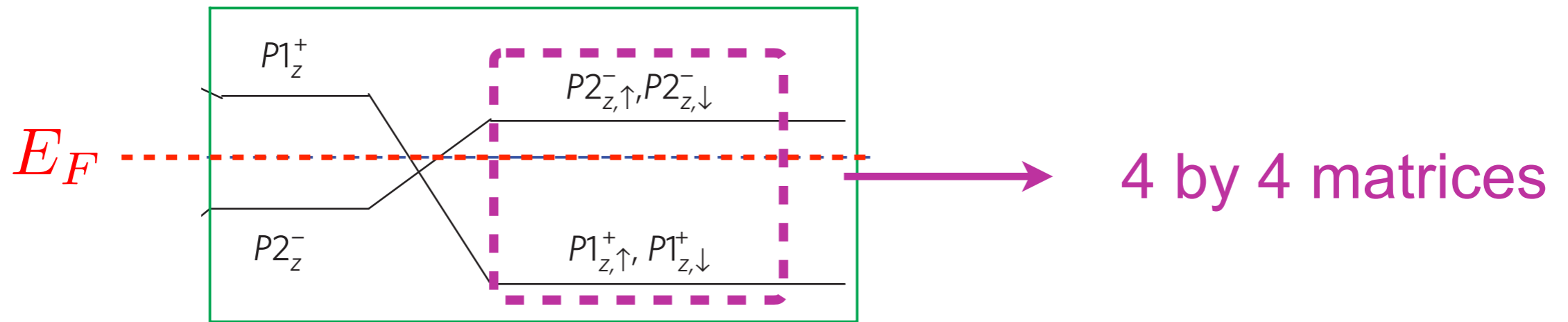
Band inversion due to strong SOC

Two bands near the Fermi energy are important





Two bands near the Fermi energy are important



$H_0(\mathbf{k})$

$$= \begin{pmatrix} \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & 0 & -iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) \\ 0 & \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & A_2(\sin k_x + i \sin k_y) & -iA_1 \sin k_z \\ iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) & 0 \\ A_2(\sin k_x + i \sin k_y) & iA_1 \sin k_z & 0 & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) \end{pmatrix}$$

**basis:**  $(|P1_z^+, \uparrow\rangle, |P1_z^+, \downarrow\rangle, |P2_z^-, \uparrow\rangle, |P2_z^-, \downarrow\rangle)$

“Effective Hamiltonian for 3D TI”

The Hamiltonian can be written in the Gamma matrices:

$$\begin{pmatrix} \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & 0 & -iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) \\ 0 & \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & A_2(\sin k_x + i \sin k_y) & -iA_1 \sin k_z \\ iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) & 0 \\ A_2(\sin k_x + i \sin k_y) & iA_1 \sin k_z & 0 & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) \end{pmatrix}$$

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$$= \epsilon_0 \mathbf{1}_{4 \times 4} + \sum_{a=1}^5 d^a \Gamma^a$$

cf. 2D toy model

$$H = \mathbf{d} \cdot \boldsymbol{\sigma}$$

$$\mathbf{d} = (m, k_x, k_y)$$

$$(d^1, d^2, d^3, d^4, d^5) = (A_2 \sin k_x, A_2 \sin k_y, A_1 \sin k_z, \mathcal{M}(\mathbf{k}), 0)$$

$$\mathcal{M}(\mathbf{k}) = M - 2B_1 - 4B_2 + 2B_1 \cos k_z + 2B_2(\cos k_x + \cos k_y)$$

$$\Gamma^1 = \begin{pmatrix} 0 & \sigma^x \\ \sigma^x & 0 \end{pmatrix} \quad \Gamma^2 = \begin{pmatrix} 0 & \sigma^y \\ \sigma^y & 0 \end{pmatrix} \quad \Gamma^3 = \begin{pmatrix} 0 & -i\mathbf{1} \\ -i\mathbf{1} & 0 \end{pmatrix}$$

$$\Gamma^4 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad \Gamma^5 = \begin{pmatrix} 0 & \sigma^z \\ \sigma^z & 0 \end{pmatrix}$$

The Hamiltonian can be written in the Gamma matrices:

$$\begin{pmatrix} \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & 0 & -iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) \\ 0 & \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & A_2(\sin k_x + i \sin k_y) & -iA_1 \sin k_z \\ iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) & 0 \\ A_2(\sin k_x + i \sin k_y) & iA_1 \sin k_z & 0 & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) \end{pmatrix}$$

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$$d_5 = 0$$

(see later discussion)

The Hamiltonian can be written in the Gamma matrices:

$$\begin{pmatrix} \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & 0 & -iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) \\ 0 & \epsilon_0(\mathbf{k}) + \mathcal{M}(\mathbf{k}) & A_2(\sin k_x + i \sin k_y) & -iA_1 \sin k_z \\ iA_1 \sin k_z & A_2(\sin k_x - i \sin k_y) & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) & 0 \\ A_2(\sin k_x + i \sin k_y) & iA_1 \sin k_z & 0 & \epsilon_0(\mathbf{k}) - \mathcal{M}(\mathbf{k}) \end{pmatrix}$$

$$= \epsilon_0 \mathbf{1}_{4 \times 4} + \sum_{a=1}^5 d^a \Gamma^a$$

important for  
topological state

cf. 2D toy model

$$H = \mathbf{d} \cdot \boldsymbol{\sigma}$$

$$\mathbf{d} = (m, k_x, k_y)$$

$$(d^1, d^2, d^3, d^4, d^5) = (A_2 \sin k_x, A_2 \sin k_y, A_1 \sin k_z, \mathcal{M}(\mathbf{k}), 0)$$

$$\mathcal{M}(\mathbf{k}) = M - 2B_1 - 4B_2 + 2B_1 \cos k_z + 2B_2(\cos k_x + \cos k_y)$$

$$\Gamma^1 = \begin{pmatrix} 0 & \sigma^x \\ \sigma^x & 0 \end{pmatrix} \quad \Gamma^2 = \begin{pmatrix} 0 & \sigma^y \\ \sigma^y & 0 \end{pmatrix} \quad \Gamma^3 = \begin{pmatrix} 0 & -i\mathbf{1} \\ -i\mathbf{1} & 0 \end{pmatrix}$$

$$\Gamma^4 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad \Gamma^5 = \begin{pmatrix} 0 & \sigma^z \\ \sigma^z & 0 \end{pmatrix}$$

## Partition function (given by path integral)

$$S_0 = \int d^4x \psi^\dagger(x) [i\partial_t - H_0] \psi(x)$$

$$\longrightarrow Z_0 = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger e^{iS_0}$$

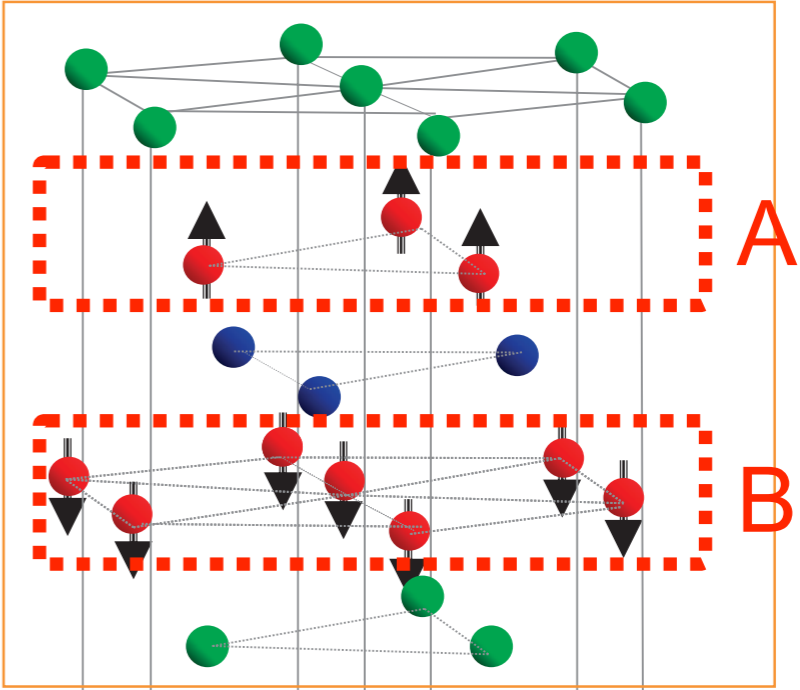
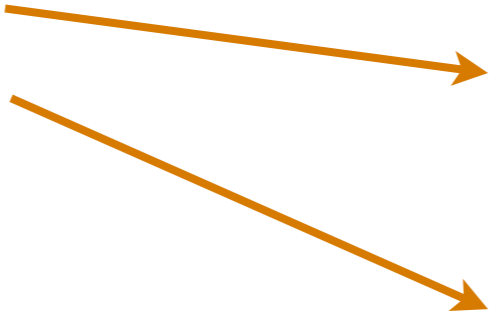
$\psi(x)$  : wavefunction of electron

$$\sim (|P1_z^+, \uparrow\rangle, |P1_z^+, \downarrow\rangle, |P2_z^-, \uparrow\rangle, |P2_z^-, \downarrow\rangle)^T$$

Now we introduce *antiferromagnetism (AFM)* by hand  
( $\mathcal{T}$  violation)

R. Li et al. '10

Suppose electrons at Bi  
are AFM order



- Bi(Fe)
- Se1
- Se2

Now we introduce *antiferromagnetism (AFM)* by hand  
 (  $\mathcal{T}$  violation)

R. Li et al. '10

$$\mathcal{H}_{\text{int}} = \frac{UV}{N} \int d^3x (n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow})$$

“Hubbard term”

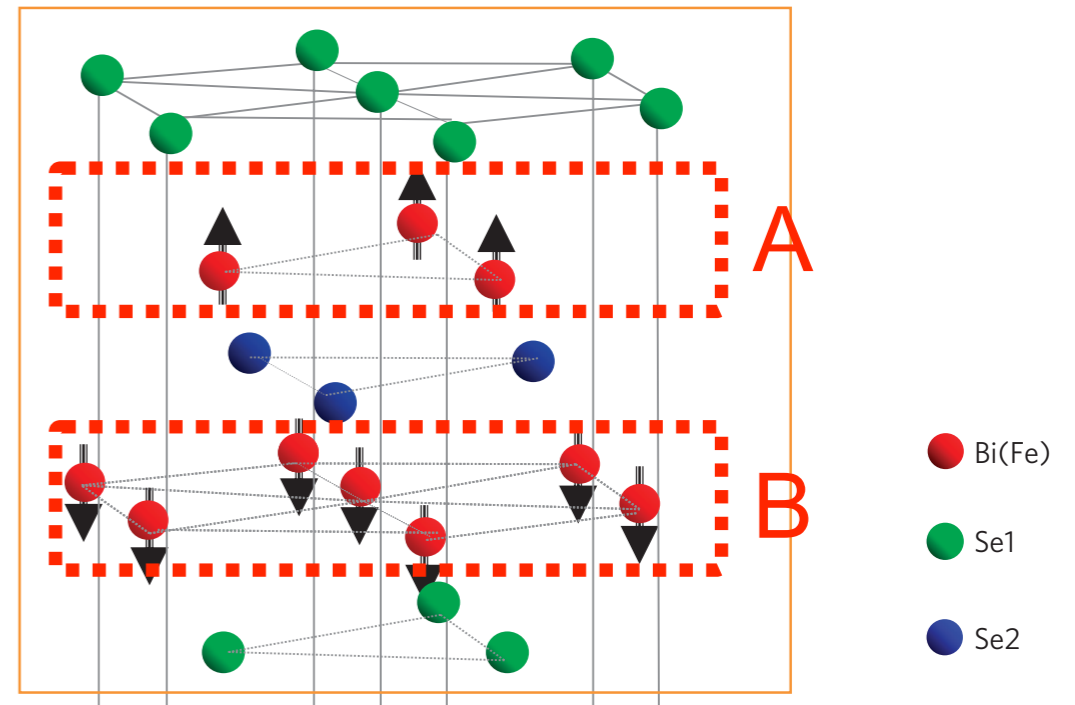
$U$  : parameter to give AFM

$V$  : volume

$N$  : number of site

$$n_{A\sigma} = \psi_{A\sigma}^\dagger \psi_{A\sigma}$$

$$n_{B\sigma} = \psi_{B\sigma}^\dagger \psi_{B\sigma}$$





Now we introduce *antiferromagnetism (AFM)* by hand  
 (  $\mathcal{T}$  violation)

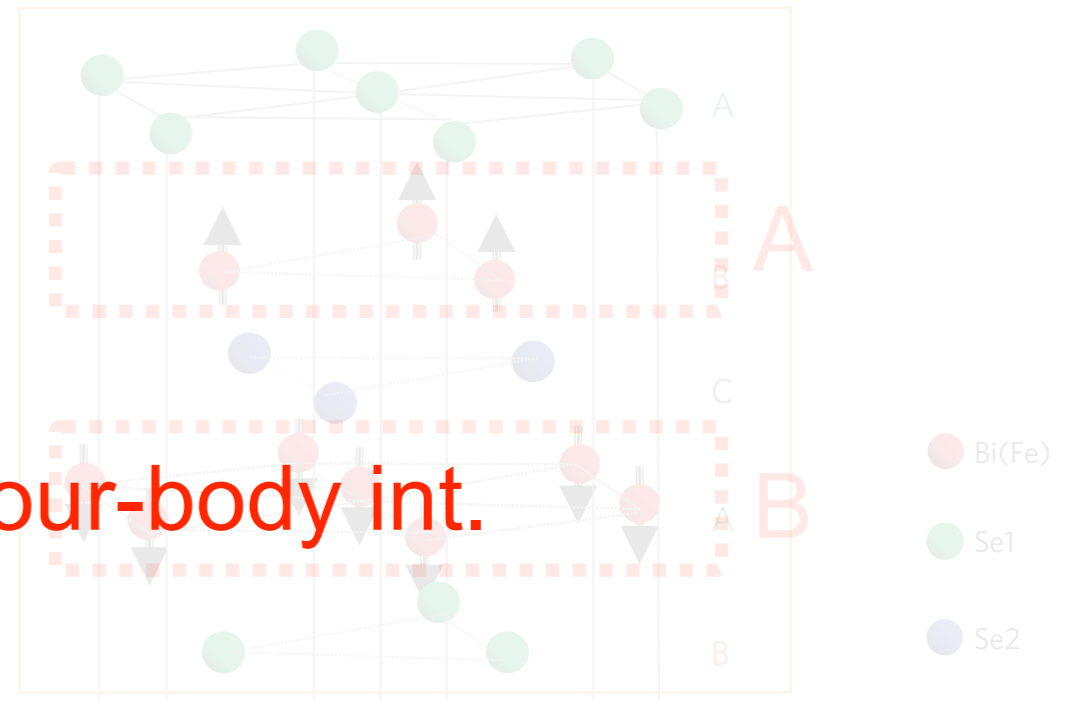
R. Li et al. '10

$$\mathcal{H}_{\text{int}} = \frac{UV}{N} \int d^3x (n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow})$$

“Hubbard term”

$U$ : parameter to give AFM

Difficult to handle since they're four-body int.



$V$  : volume  
 $N$  : number of site

$$n_{A\sigma} = \psi_{A\sigma}^\dagger \psi_{A\sigma}$$

$$n_{B\sigma} = \psi_{B\sigma}^\dagger \psi_{B\sigma}$$

## Hubbard-Stratonovich (HS) transformation

$$\mathcal{H}_{\text{int}} = \frac{UV}{N} \int d^3x (n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow})$$

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HS transformation

- A dynamical scalar  $\phi$  that gives  $\Gamma^5 d_5$  ( $d_5 = \phi$ )
- Mass term of  $\phi$

This can be understood from

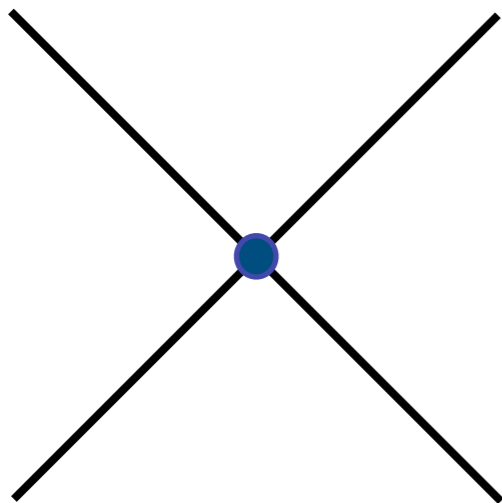
HS transformation

~ Inverse of integrating out a scalar

This can be understood from

HS transformation

$\sim$  Inverse of integrating out a scalar

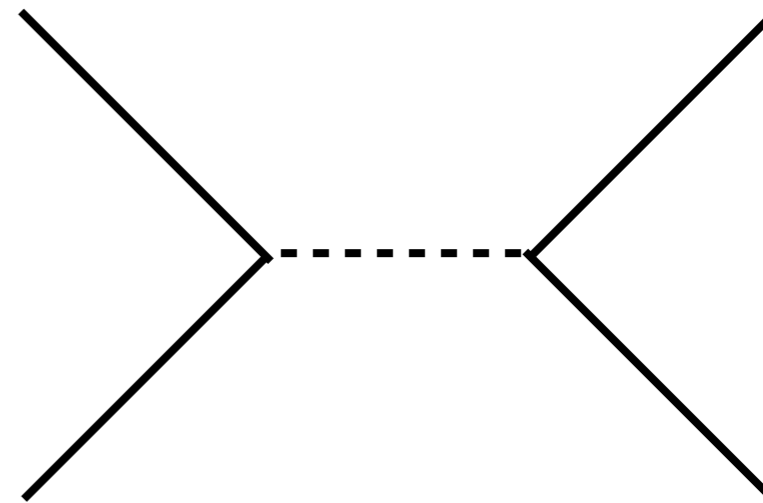


$$n_{A\uparrow}n_{A\downarrow}, n_{B\uparrow}n_{B\downarrow}$$
$$(\psi_{\uparrow}^{\dagger}\psi_{\uparrow}\psi_{\downarrow}^{\dagger}\psi_{\downarrow})$$

Four Fermi int.



Integrate out  $\phi$



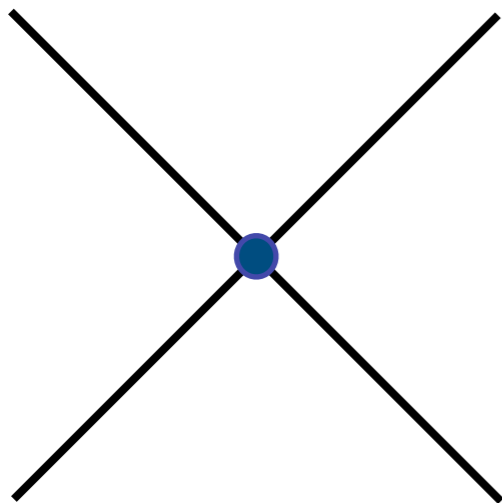
$$\phi\psi_{\uparrow}^{\dagger}\psi_{\uparrow}, \phi\psi_{\downarrow}^{\dagger}\psi_{\downarrow}$$

Yukawa int.

This can be understood from

HS transformation

$\sim$  Inverse of integrating out a scalar



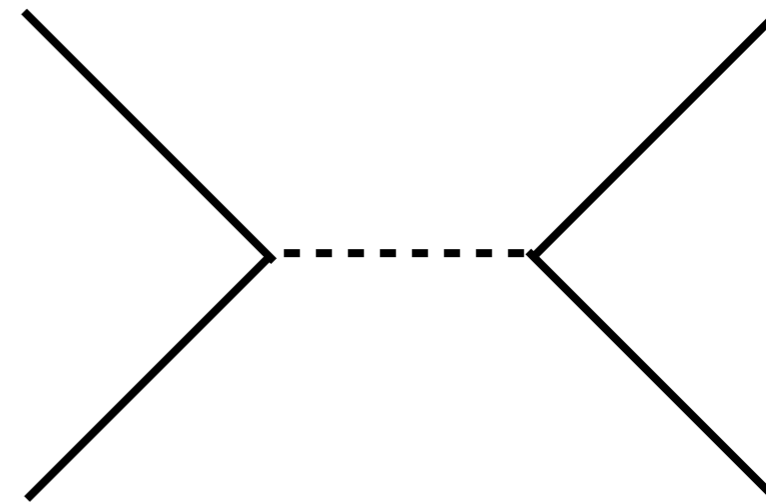
$$n_{A\uparrow}n_{A\downarrow}, n_{B\uparrow}n_{B\downarrow}$$
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Four Fermi int.

HS transformation



Integrate out  $\phi$



$$\phi\psi_{\uparrow}^{\dagger}\psi_{\uparrow}, \phi\psi_{\downarrow}^{\dagger}\psi_{\downarrow}$$

Yukawa int.

# Hubbard-Stratonovich (HS) transformation

$$\mathcal{H}_{\text{int}} = \frac{UV}{N} \int d^3x (n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow})$$



HS transformation

- A dynamical scalar  $\phi$  that gives  $\Gamma^5 d_5$  ( $d_5 = \phi$ )

- Mass term of  $\phi$   missed in [Sekine, Nomura '16](#)  
[Sekine, Nomura '20](#)  
[Schütte-Engel '21](#)

(confirmed by private communication  
with Sekine-san)

## Hubbard-Stratonovich (HS) transformation

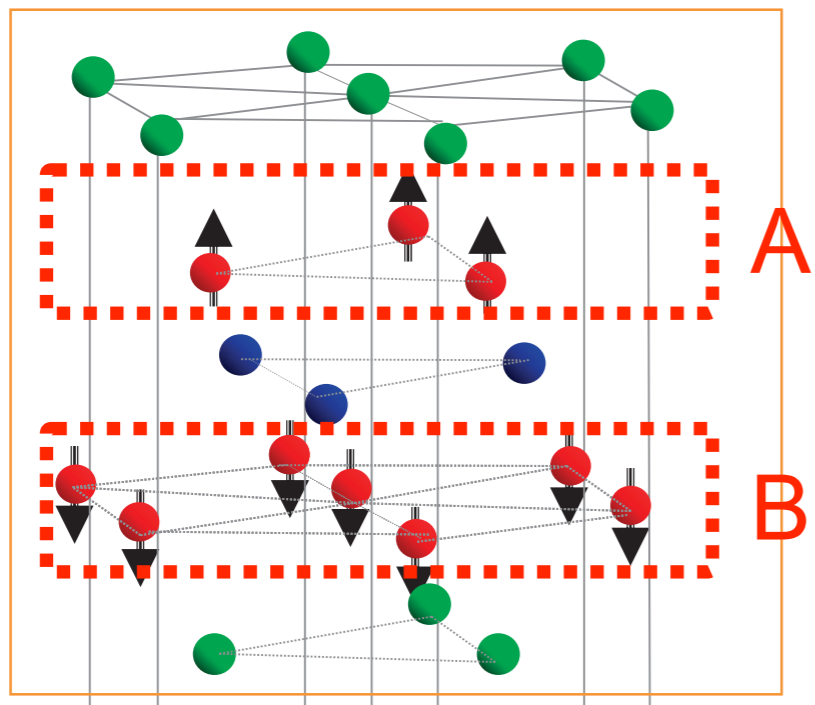
$$\mathcal{H}_{\text{int}} = \frac{UV}{N} \int d^3x (n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow})$$



HS transformation

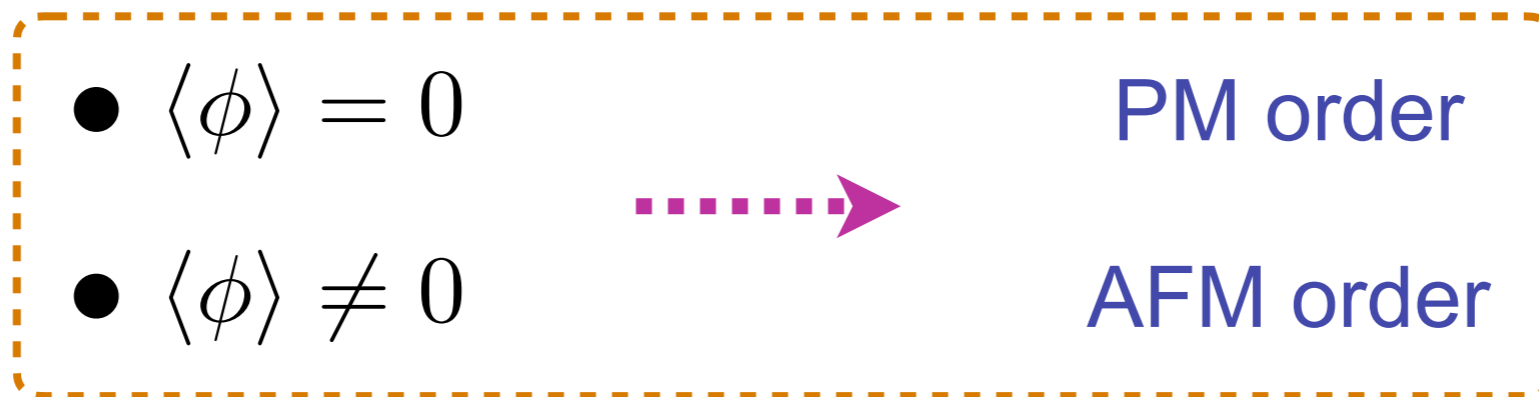
- A dynamical scalar  $\phi$  that gives  $\Gamma^5 d_5$  ( $d_5 = \phi$ )
- Mass term of  $\phi$
- VEV of  $\phi$  is the order parameter of the AFM





- Bi(Fe)
- Se1
- Se2

$$\langle \phi \rangle \sim \langle S_A \rangle = - \langle S_B \rangle$$



PM (paramagnetic)

## Partition function (TI + AFM)

$$Z = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger \mathcal{D}\phi e^{iS + iS_\phi^{\text{mass}}}$$

$$S = \int d^4x \psi^\dagger(x) [i\partial_t - H] \psi(x)$$

$$S_\phi^{\text{mass}} = - \int d^4x M_\phi^2 \phi^2$$

$$H = H_0 + \delta H$$

$$M_\phi^2 = \int \frac{d^3k}{(2\pi)^3} \frac{2}{U}$$

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$\Gamma^5 \phi$   
↓

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$$H = H_0 + \delta H$$

$\Gamma^5 \phi$   
↓  
⊞

$$M_\phi^2 = \int \frac{d^3k}{(2\pi)^3} \frac{2}{U}$$

Integrate out  $\psi, \psi^\dagger$



Effective action for  $\phi$

## Effective potential for $\phi$

KI '21

$$V_\phi = -2 \int \frac{d^3 k}{(2\pi)^3} (\sqrt{|d_0|^2 + \phi^2} - |d_0|) + M_\phi^2 \phi^2$$

$$|d_0|^2 = \sum_{a=1}^4 |d^a|^2$$
$$M_\phi^2 = \int \frac{d^3 k}{(2\pi)^3} \frac{2}{U}$$

## Effective potential for $\phi$

KI '21

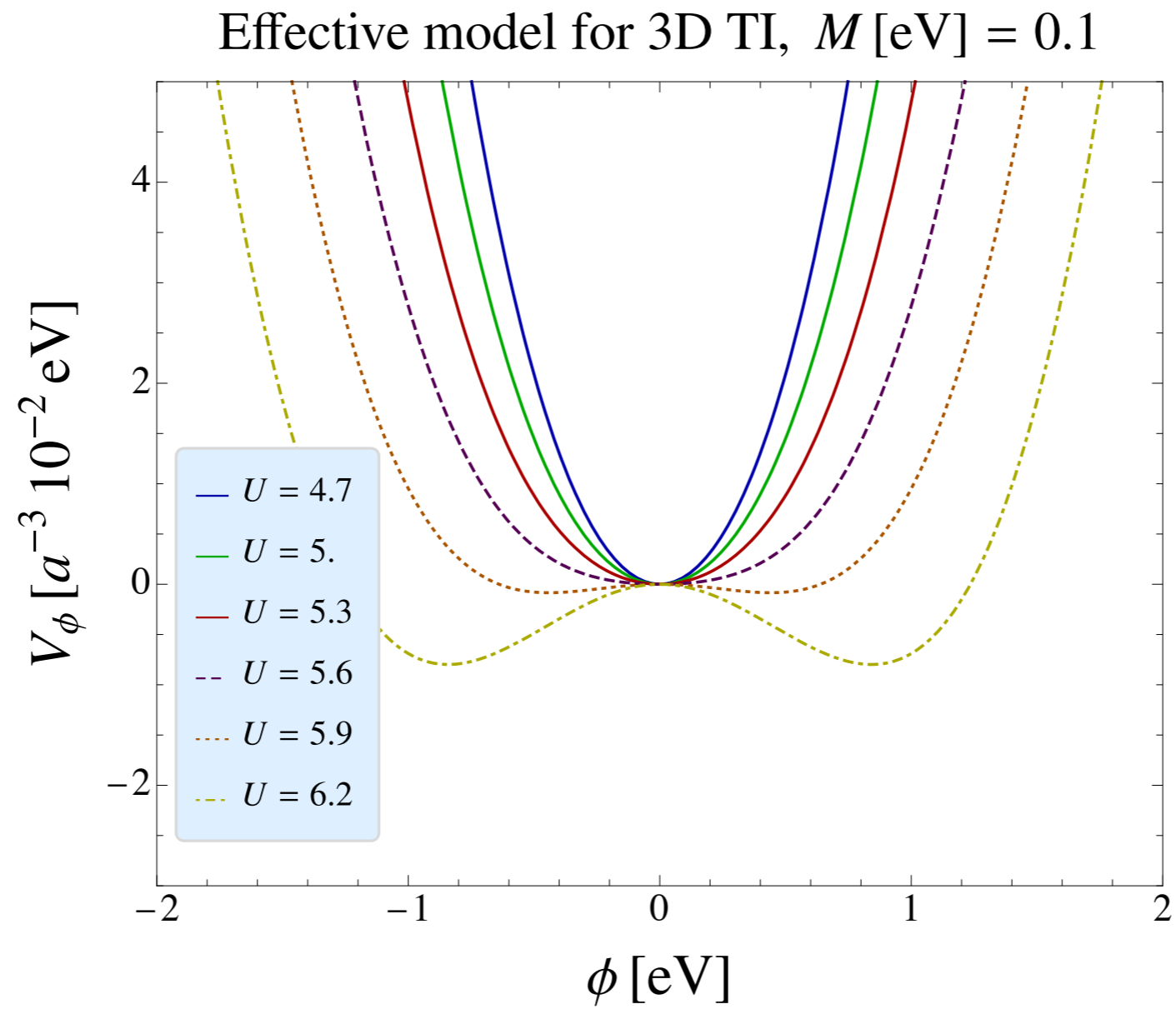
$$V_\phi = -2 \int \frac{d^3 k}{(2\pi)^3} (\sqrt{|d_0|^2 + \phi^2} - |d_0|) + M_\phi^2 \phi^2$$

Negative potential



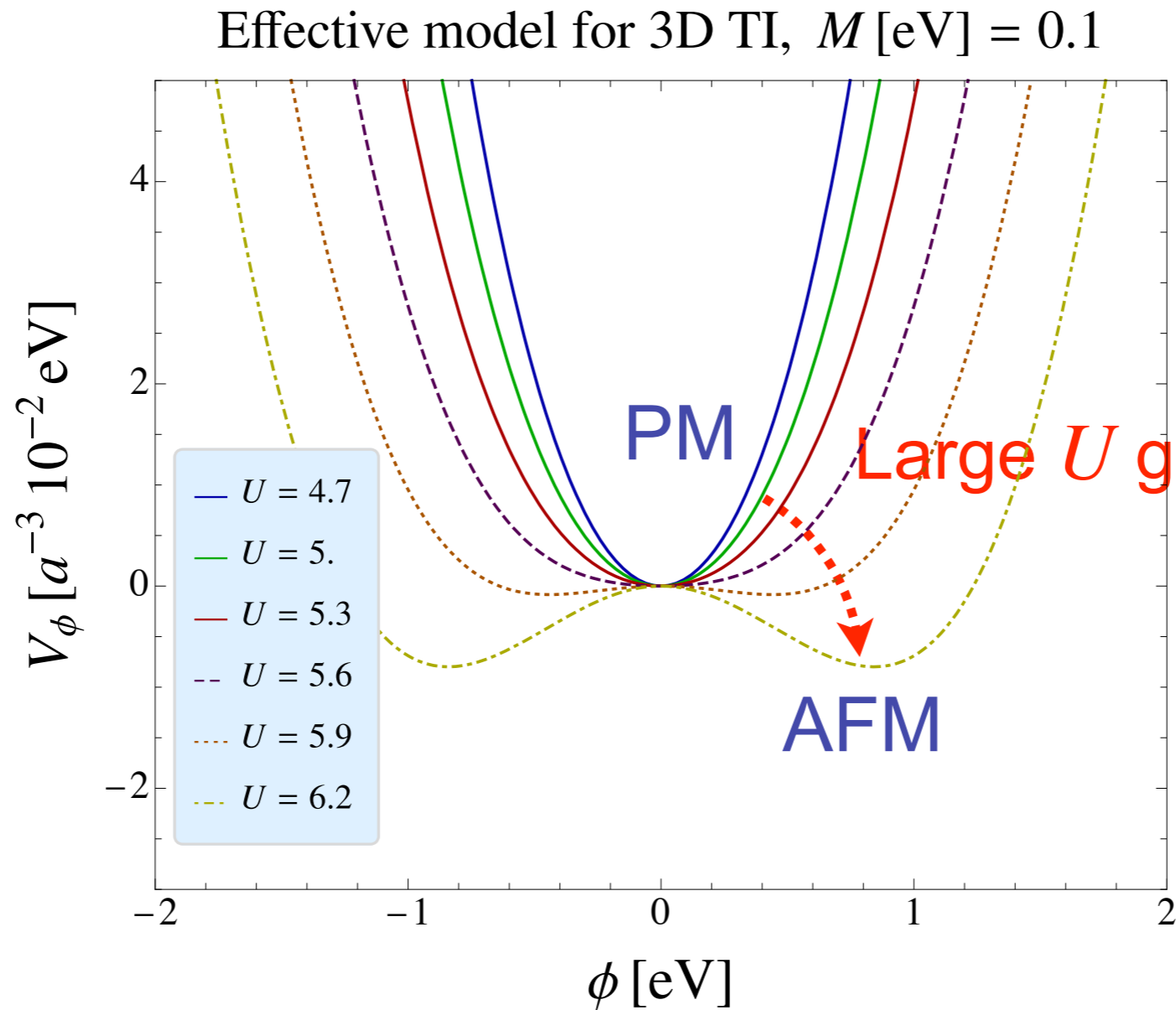
The mass term stabilizes the potential

$$|d_0|^2 = \sum_{a=1}^4 |d^a|^2$$
$$M_\phi^2 = \int \frac{d^3 k}{(2\pi)^3} \frac{2}{U}$$



$$A_1 = A_2 = 1$$

$$B_1 = B_2 = -0.5$$



$$A_1 = A_2 = 1$$

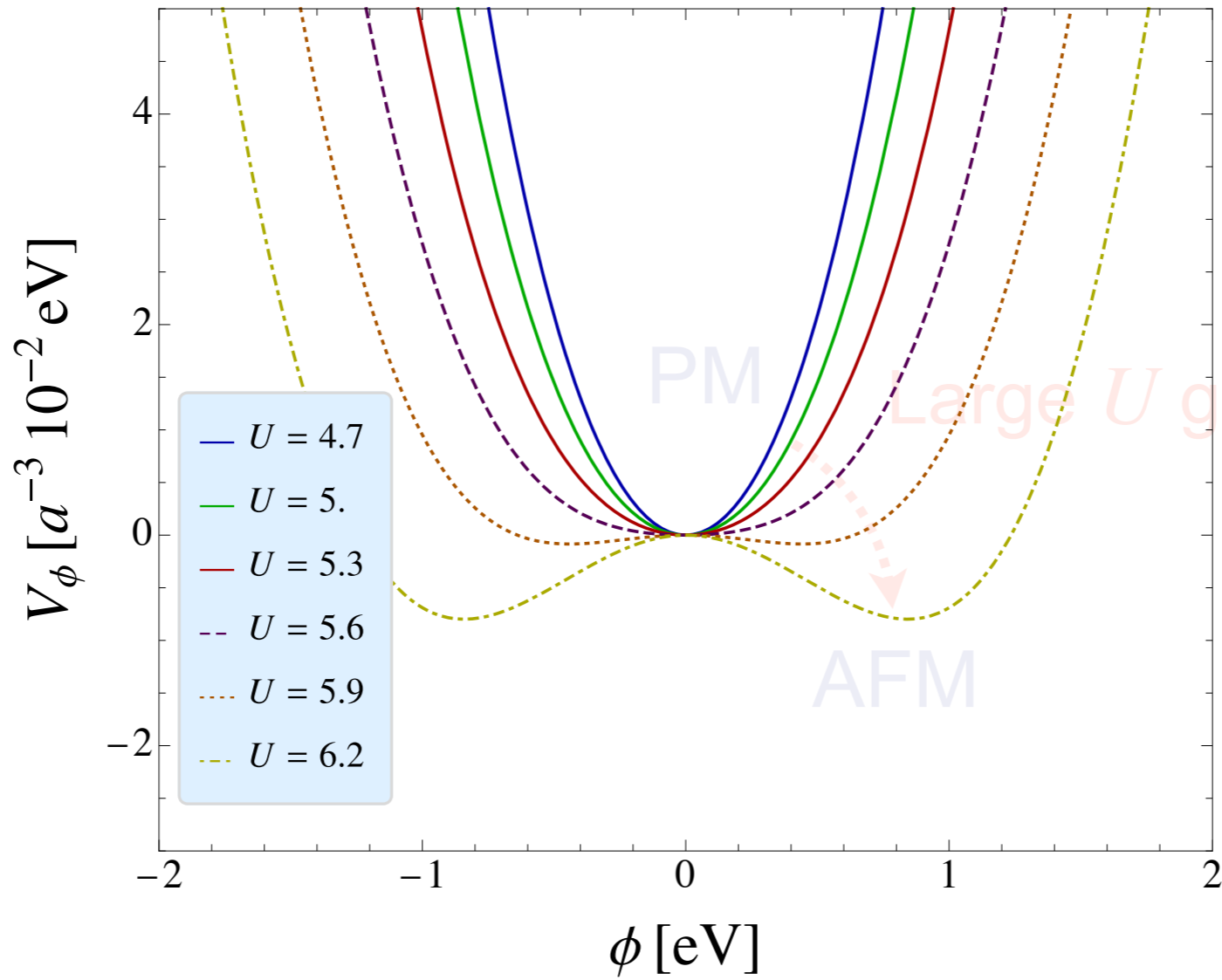
$$B_1 = B_2 = -0.5$$

Phase transition from PM to AFM

$$\therefore M_\phi^2 \propto 1/U$$



Effective model for 3D TI,  $M$  [eV] = 0.1



$$A_1 = A_2 = 1$$

$$B_1 = B_2 = -0.5$$

**Where is axion?**

$\theta$  can be computed from Hamiltonian:

- $$\theta = \frac{1}{4\pi} \int d^3k \frac{2|d| + d^4}{(|d| + d^4)^2 |d|^3} \epsilon^{ijkl} d^i \partial_{k_x} d^j \partial_{k_y} d^k \partial_{k_z} d^l$$

R. Li et al. '10

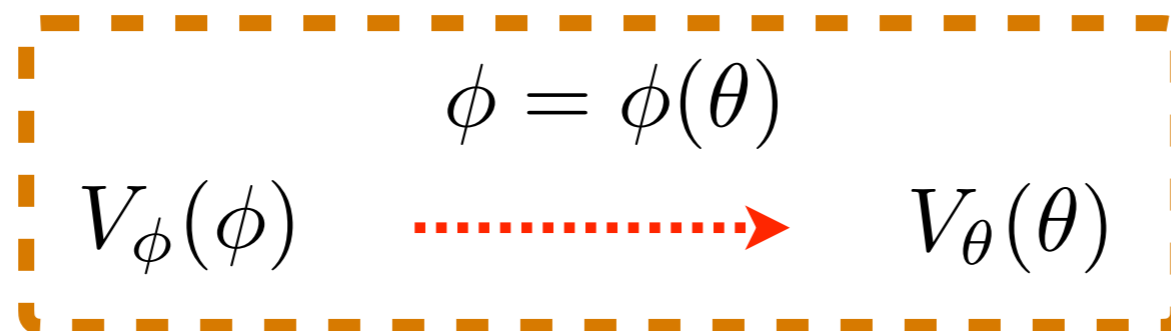
- Approximately given by chiral anomaly (Fujikawa method)

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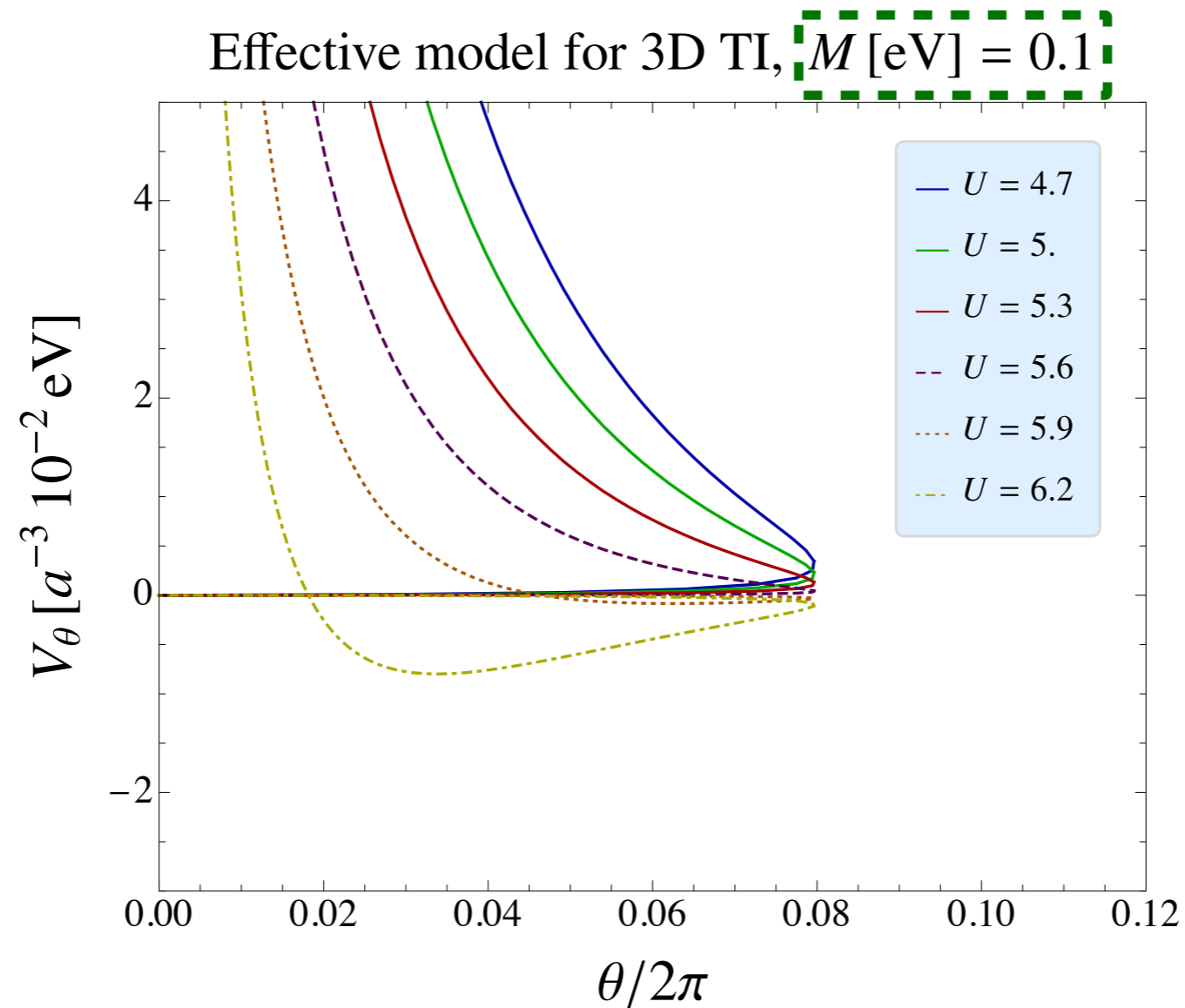
- $$\theta = \frac{1}{4\pi} \int d^3k \frac{2|d| + d^4}{(|d| + d^4)^2 |d|^3} \epsilon^{ijkl} d^i \partial_{k_x} d^j \partial_{k_y} d^k \partial_{k_z} d^l$$

R. Li et al. '10

- Approximately given by chiral anomaly (Fujikawa method)



# Effective potential in terms of $\theta$

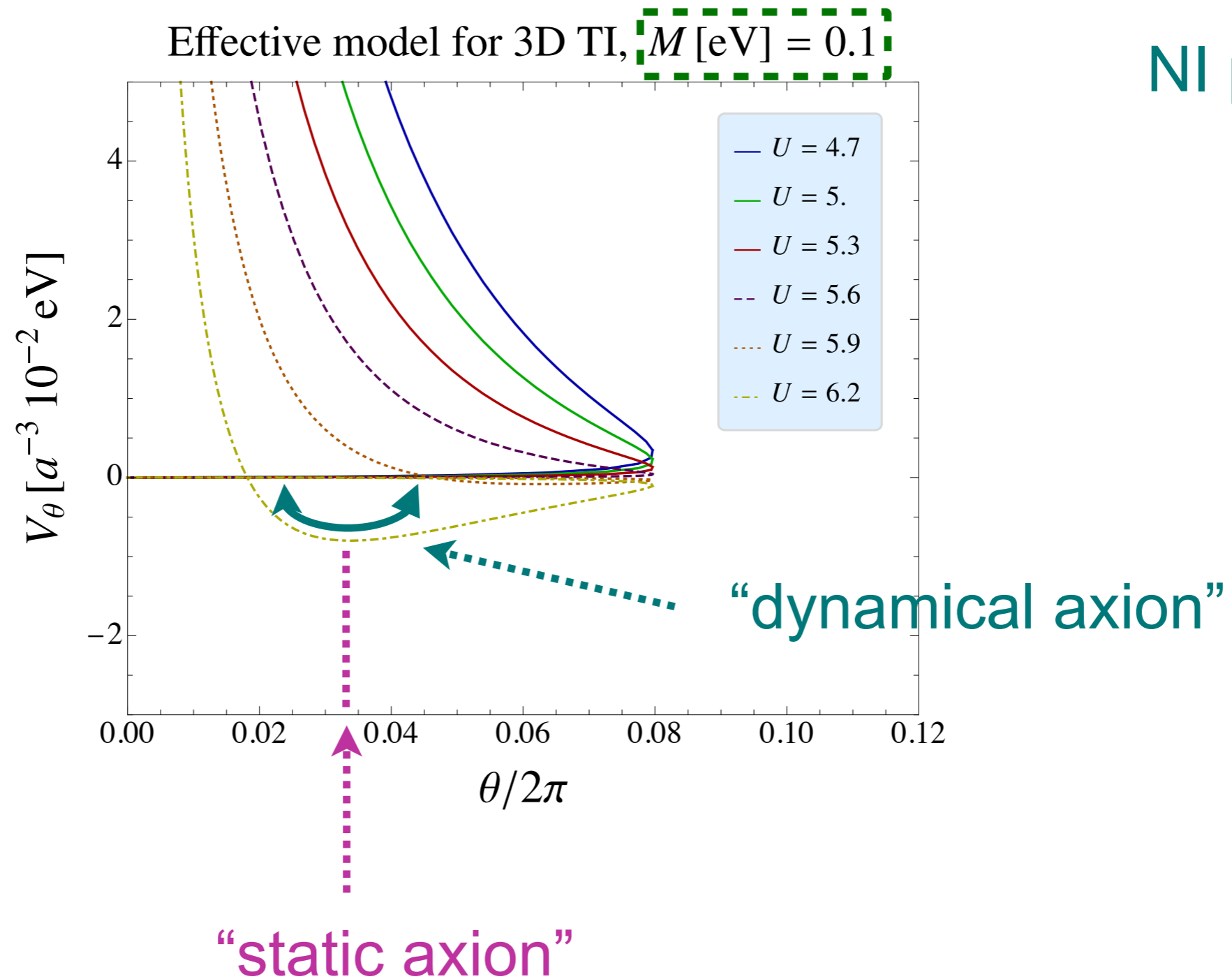


NI phase

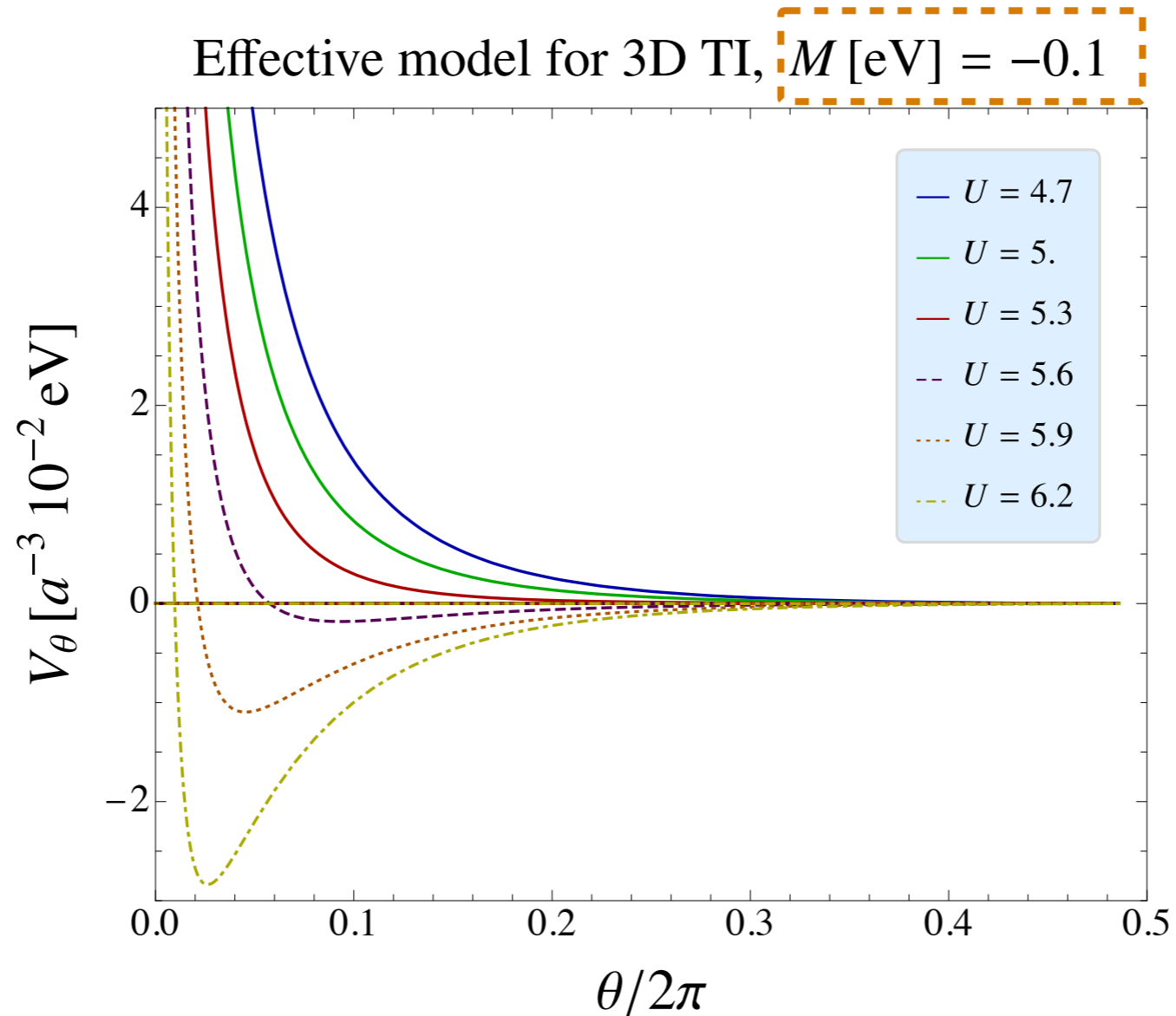
Potential minimum:

- $\theta = 0$  (small  $U$ , i.e., PM)
- $\theta \neq 0$  (large  $U$ , i.e., AFM)

# Effective potential in terms of $\theta$



# Effective potential in terms of $\theta$

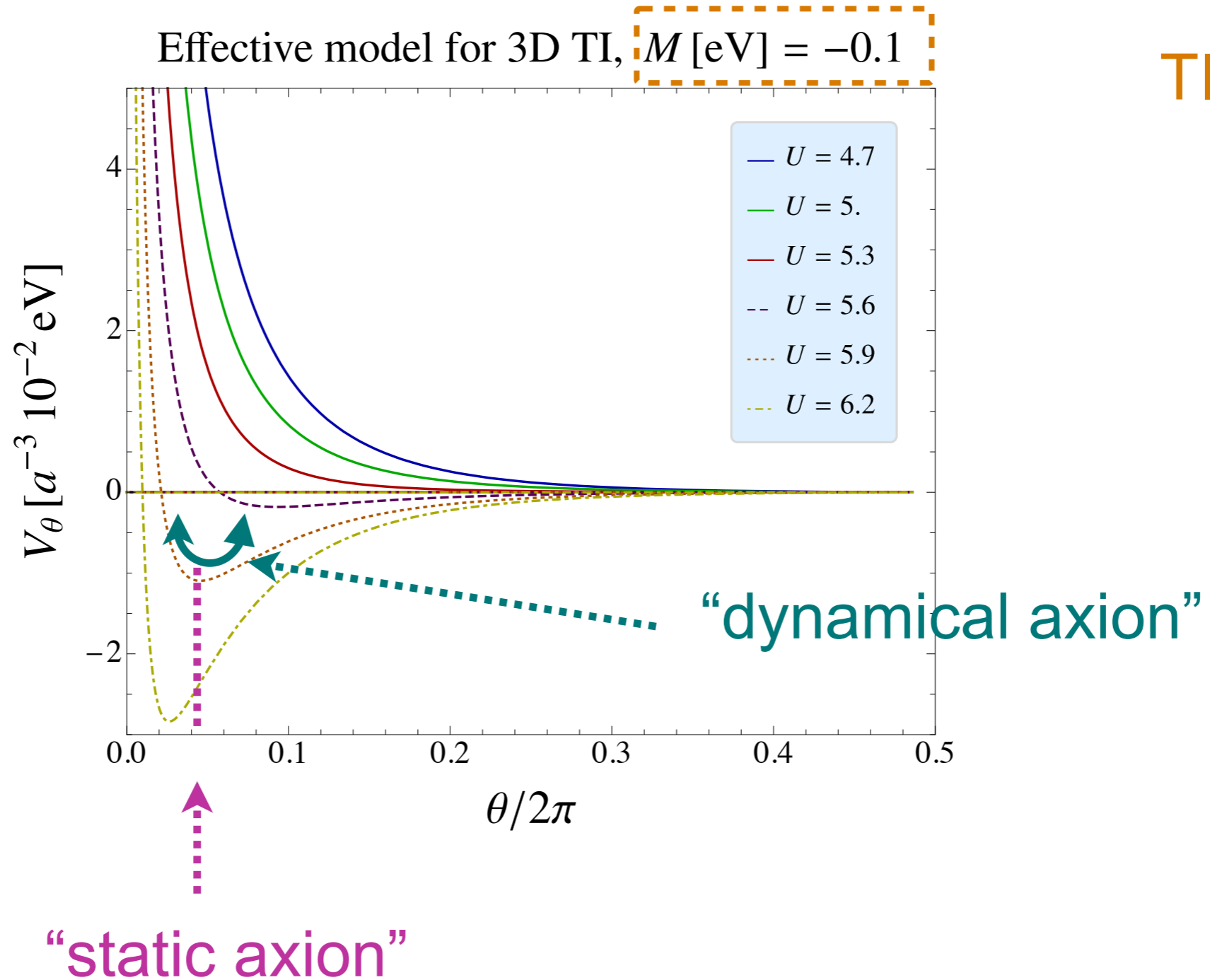


TI phase

Potential minimum:

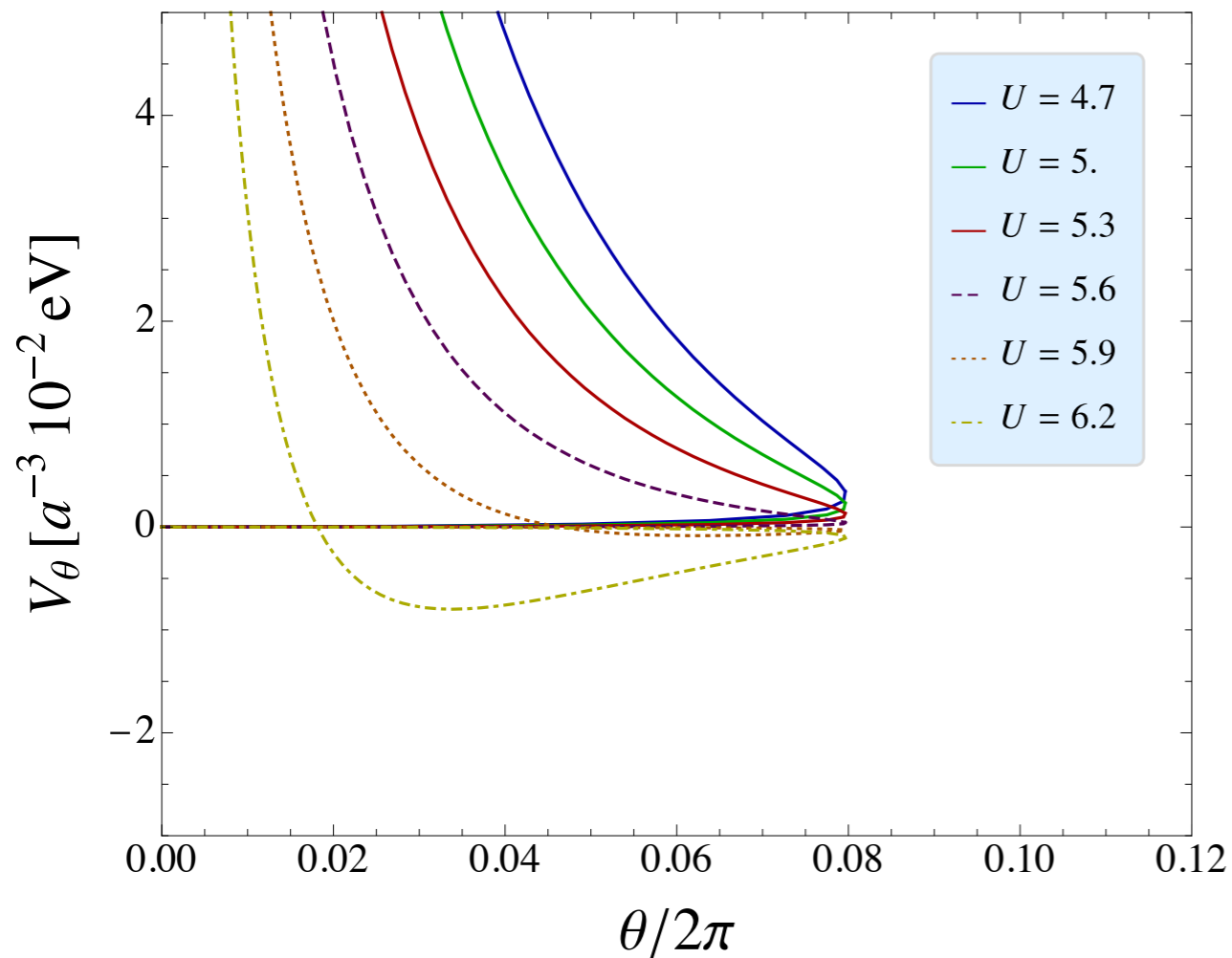
- $\theta = \pi$  (small  $U$ , i.e., PM)
- $\theta \neq 0$  (large  $U$ , i.e., AFM)

# Effective potential in terms of $\theta$

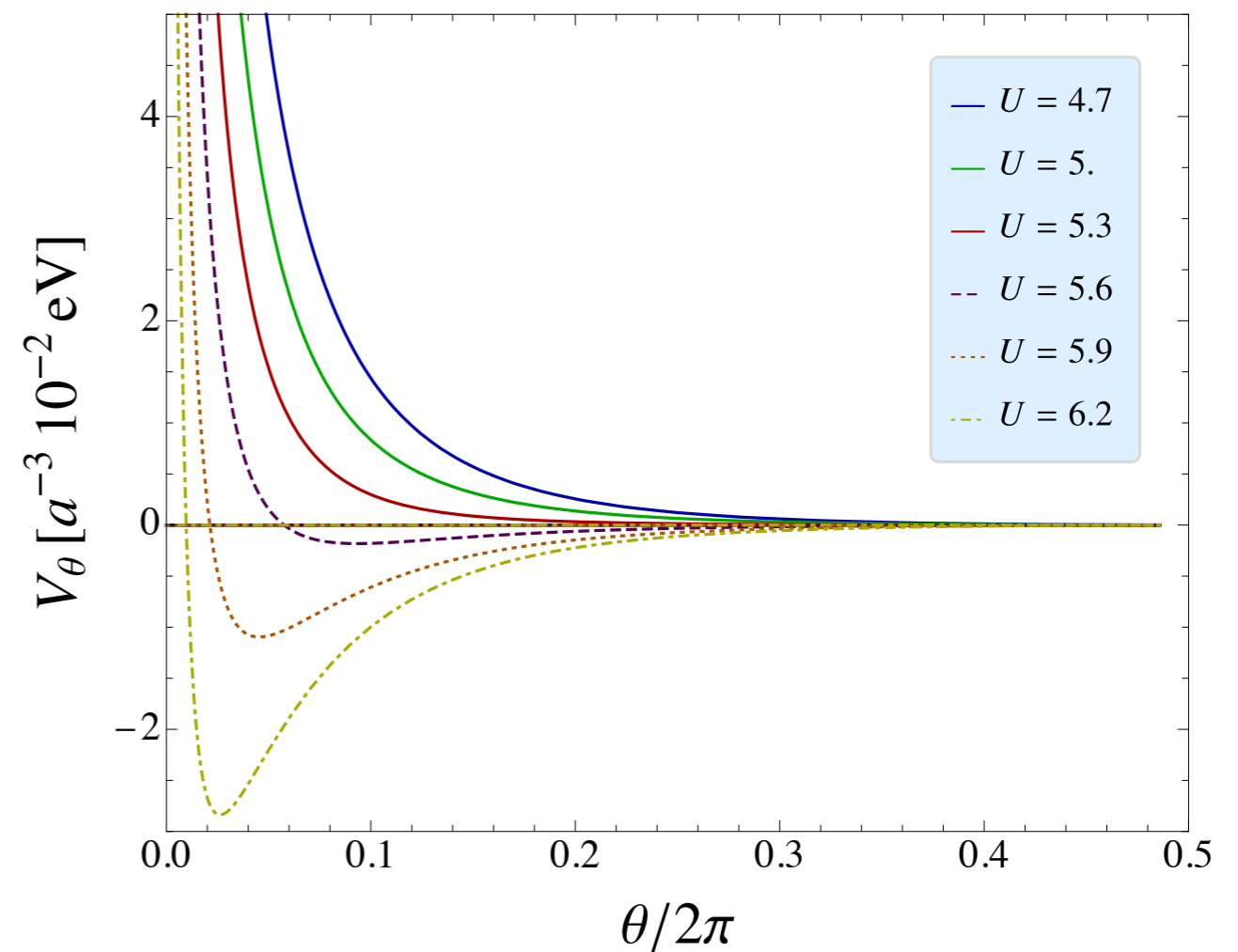


# Axion in antiferromagnetic insulators

Effective model for 3D TI,  $M$  [eV] = 0.1



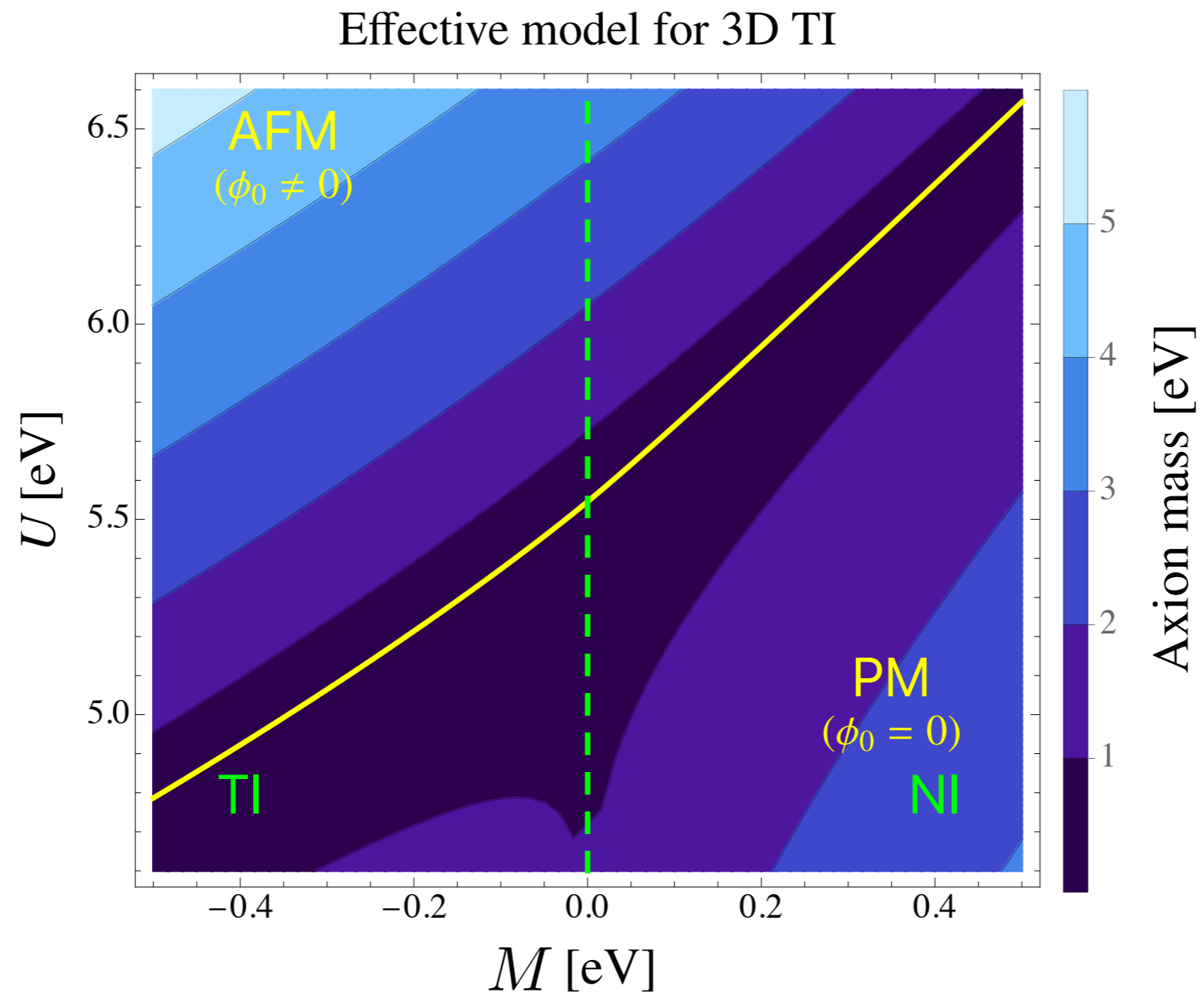
Effective model for 3D TI,  $M$  [eV] = -0.1



Dynamical axion exits in both TI and NI phases



# Axion mass



Axion mass is  $\mathcal{O}(\text{eV})$

# Axion is predicted in topological magnetic insulators

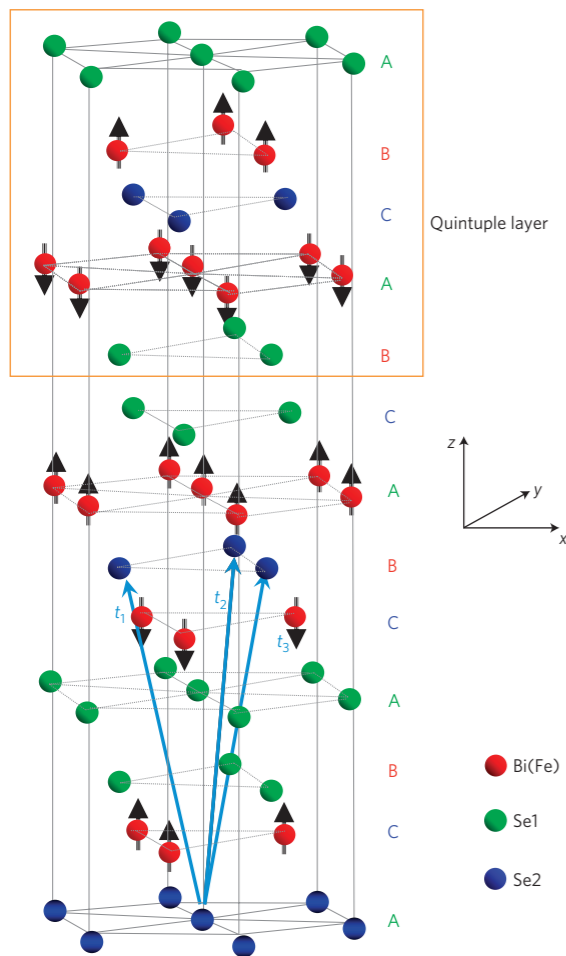
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PUBLISHED ONLINE: 7 MARCH 2010 | DOI: 10.1038/NPHYS1534

nature  
physics

## Dynamical axion field in topological magnetic insulators

Rundong Li<sup>1</sup>, Jing Wang<sup>1,2</sup>, Xiao-Liang Qi<sup>1</sup> and Shou-Cheng Zhang<sup>1\*</sup>



$\text{Bi}_2\text{Se}_3$

$$\begin{aligned}
 \mathcal{S}_{\text{tot}} &= \mathcal{S}_{\text{Maxwell}} + \mathcal{S}_{\text{topo}} + \mathcal{S}_{\text{axion}} \\
 &= \frac{1}{8\pi} \int d^3x dt \left( \epsilon \mathbf{E}^2 - \frac{1}{\mu} \mathbf{B}^2 \right) + \frac{\alpha}{4\pi^2} \int d^3x dt (\theta_0 + \delta\theta) \mathbf{E} \cdot \mathbf{B} \\
 &\quad + g^2 J \int d^3x dt [(\partial_t \delta\theta)^2 - (v_i \partial_i \delta\theta)^2 - m^2 \delta\theta^2] \quad (4)
 \end{aligned}$$

$\theta F_{\mu\nu} \tilde{F}^{\mu\nu}$

Axion mass  $\sim \mathcal{O}(\text{meV})$

# Axion is predicted in topological magnetic insulators

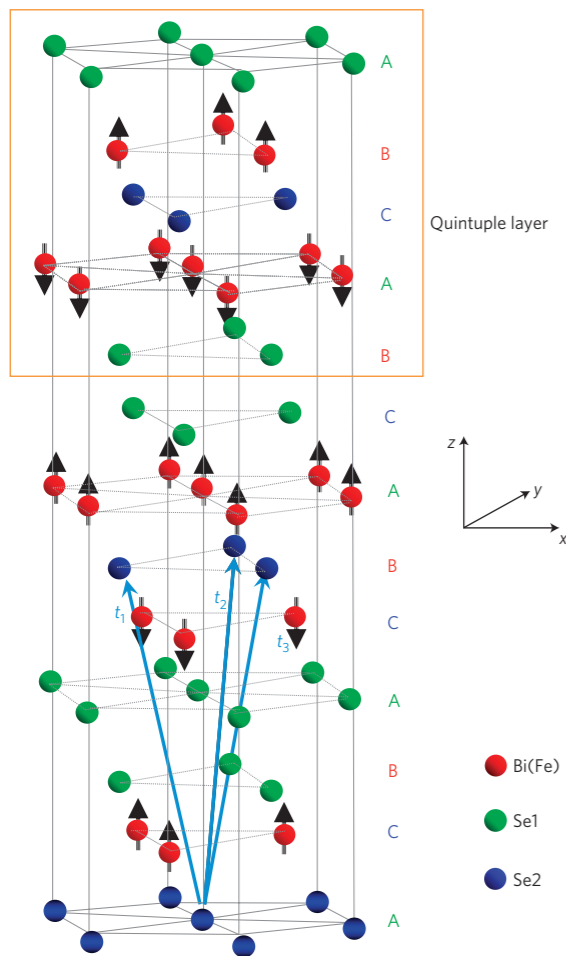
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 \end{aligned}$$

Axion mass  $\sim \mathcal{O}(\text{meV})$

?

# The thing would be ...

R. Li et al. '10

- $\langle \phi \rangle (= m_5) = 1 \text{ meV}$  is taken  
(i.e.,  $\langle \phi \rangle$  is considered to be a free parameter)

- AFM order is *assumed*

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R. Li et al. '10

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→ Axion mass  $\sim \mathcal{O}(\text{meV})$  ( $\because m_a^2 \propto m_5^2$ )

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R. Li et al. '10

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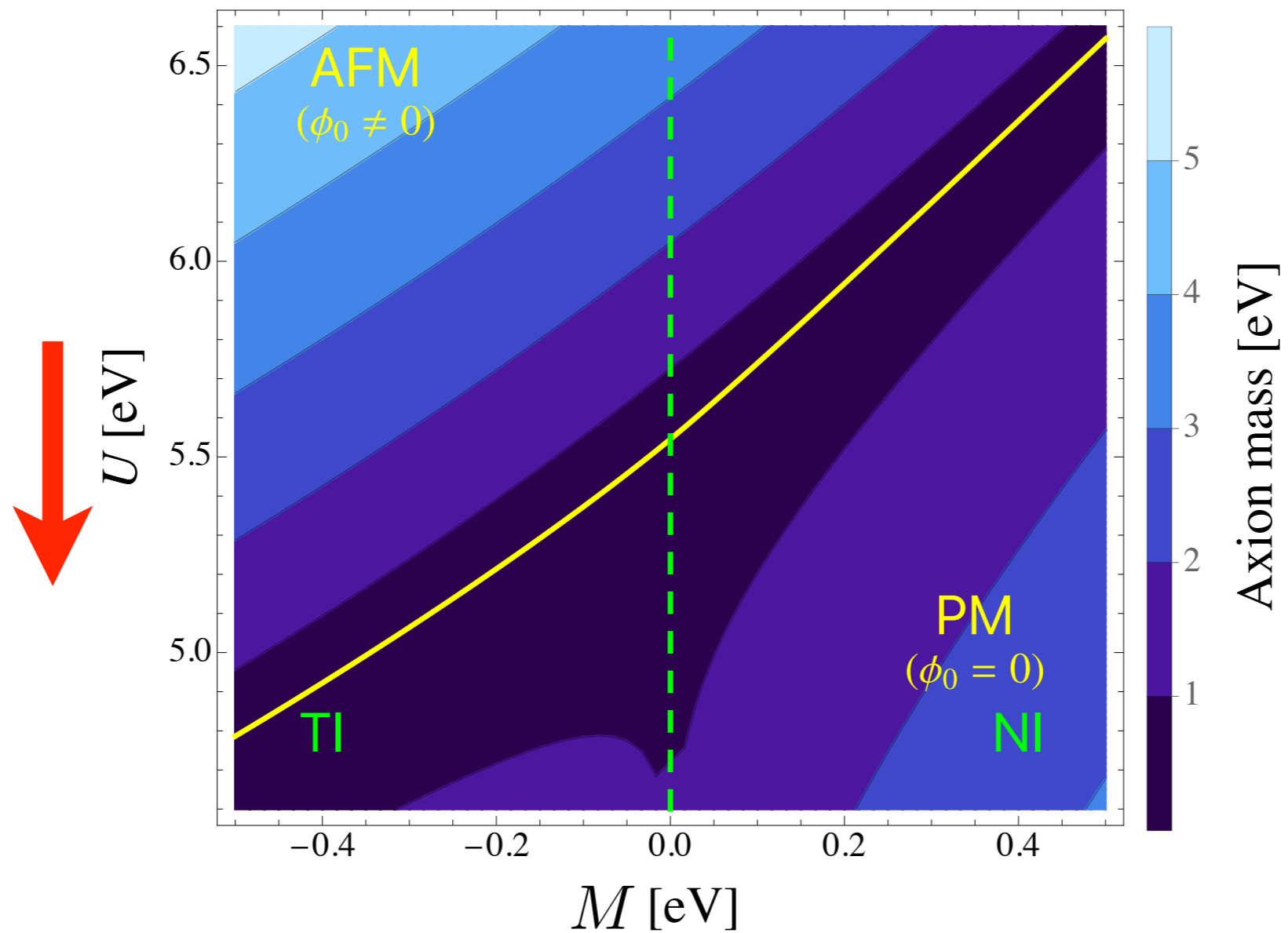
→ Axion mass  $\sim \mathcal{O}(\text{meV})$  ( $\because m_a^2 \propto m_5^2$ )

But this is not naively possible since

- AFM order is *assumed*  
 $m_5 \sim U \sim \text{eV}$  (in AFM order)

# Axion mass

Effective model for 3D TI



Suppressed  $U$   $\longrightarrow$  No AFM

# The thing would be ...

R. Li et al. '10

- $\langle \phi \rangle (= m_5) = 1 \text{ meV}$  is taken

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R. Li et al. '10

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→ Axion mass  $\sim \mathcal{O}(\text{meV})$  ( $\because m_a^2 \propto m_5^2$ )

- AFM order is *assumed*

No AFM in TI in the first place

→ Fe-doped  $\text{Bi}_2\text{Se}_3$  is considered

- Fe-doped  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$

“likely to be AFM”

(by first-principles calculation)

J.M. Zhang et al. '13

→ It looks unlikely to be realized ...

- $\text{Mn}_2\text{Bi}_2\text{Te}_5$

J. Zhang et al. '19

“rich magnetic topological quantum states”

(by first-principles calculation)

Y. Li et al. '20

## **4. Conclusions and discussion**

We have formulated static and dynamical axions in AFM TI consistently by using path integral

- Nonzero  $\langle \phi \rangle$  is obtained from the effective potential, which gives rise to AFM order and breaks  $\mathcal{T}$
- Dynamical axion appears both in TI and NI
- Axion mass is  $\lesssim \mathcal{O}(\text{eV})$

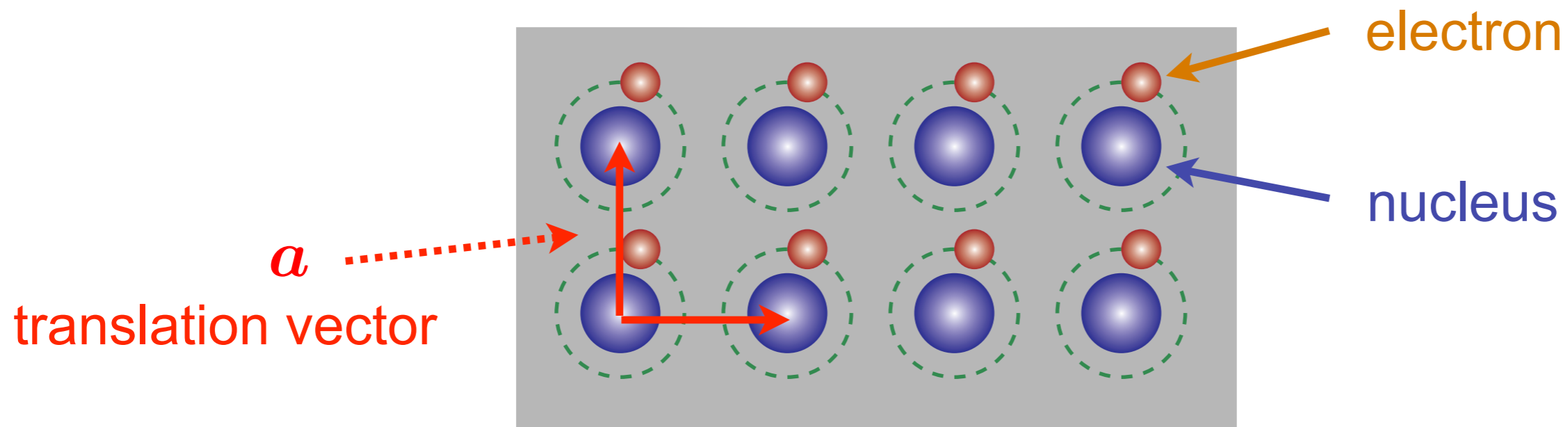
## Discussion

- How do we describe axion in  $\text{Mn}_2\text{Bi}_2\text{Te}_5$  ?
- What about axion in NI ?
- Dynamical axion in ferromagnetic state or other magnetic states?

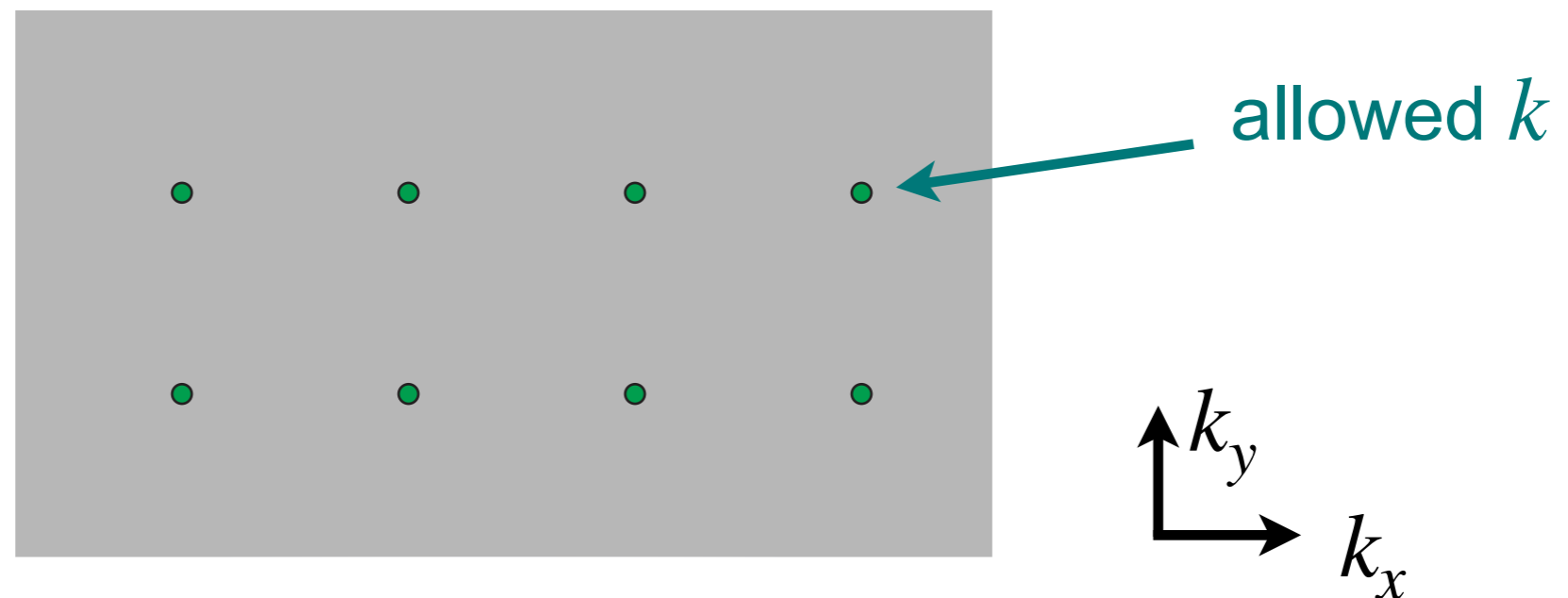
# Backups

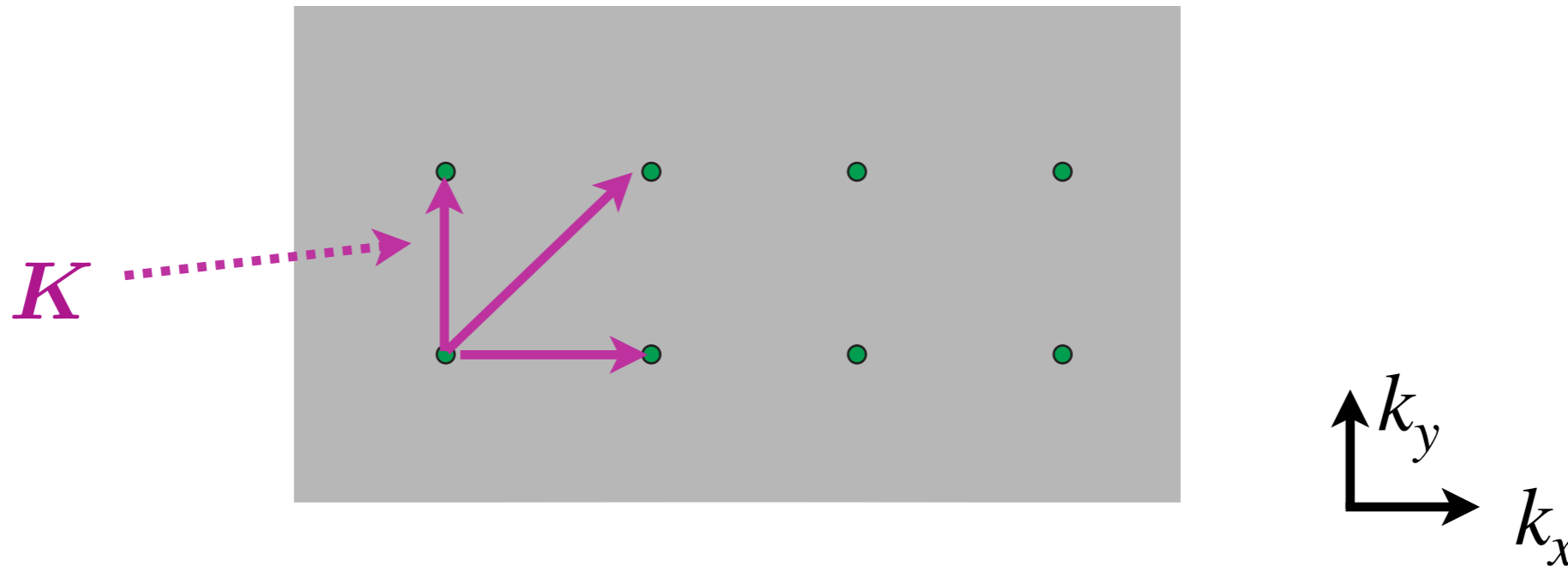
## Basics

- Wavefunction of electrons is periodic (due to the crystal structure of the material)



- Consequently there is periodicity in the wavenumber space





- Periodicity  $\boldsymbol{x} \rightarrow \boldsymbol{x} + \boldsymbol{a}$  corresponds to  $\boldsymbol{k} \rightarrow \boldsymbol{k} + \boldsymbol{K}$   
(  $\boldsymbol{K}$ : reciprocal lattice vector)
- It is enough to consider region,  $|\boldsymbol{k}| \lesssim |\boldsymbol{K}/2|$  (1st Brillouin zone)
- The wavefunction of the electrons is given by

$$\psi(\boldsymbol{x}) = u_{\boldsymbol{k}}(\boldsymbol{x}) e^{i\boldsymbol{k} \cdot \boldsymbol{x}} \quad \text{where} \quad u_{\boldsymbol{k}}(\boldsymbol{x} + \boldsymbol{a}) = u_{\boldsymbol{k}}(\boldsymbol{x})$$

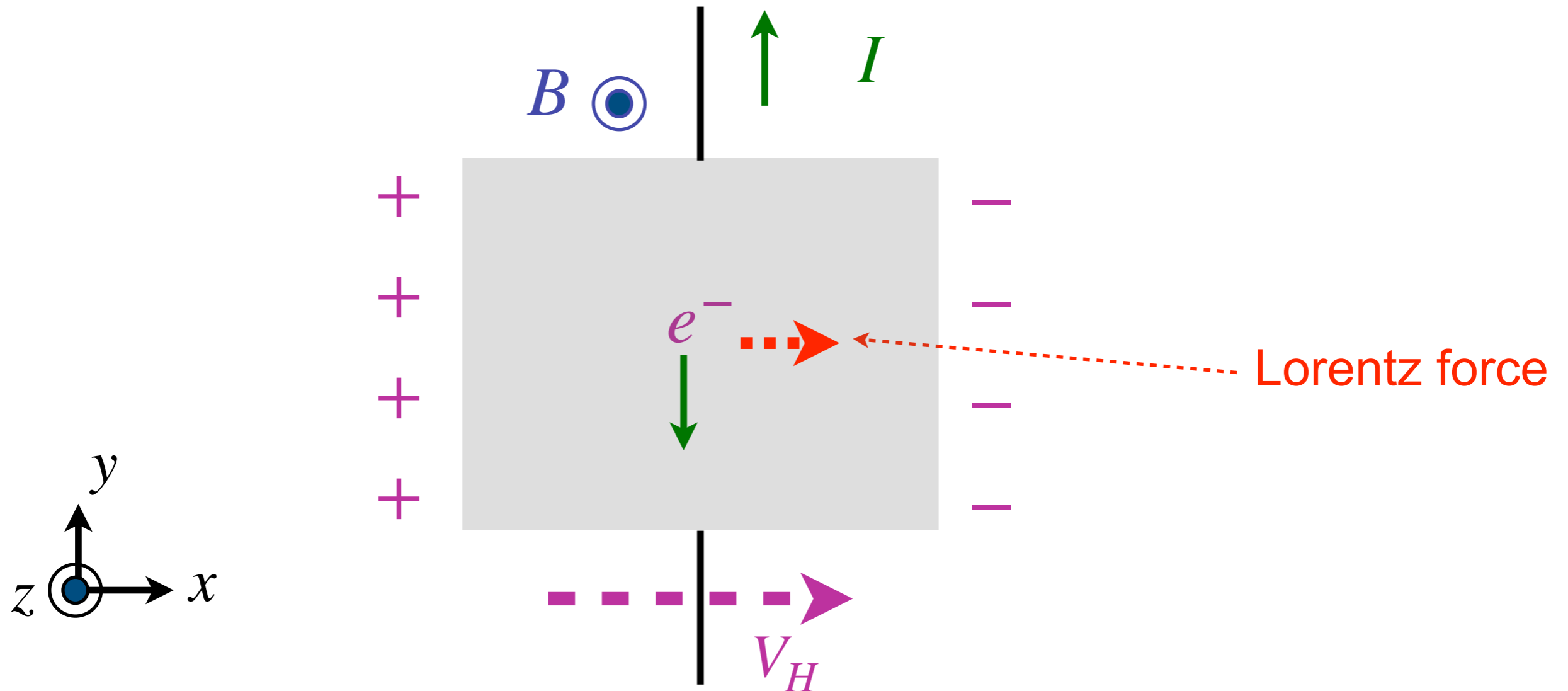
(Bloch's theorem)

*Bloch function (state)*



## Hall effect

e.g., semiconductor



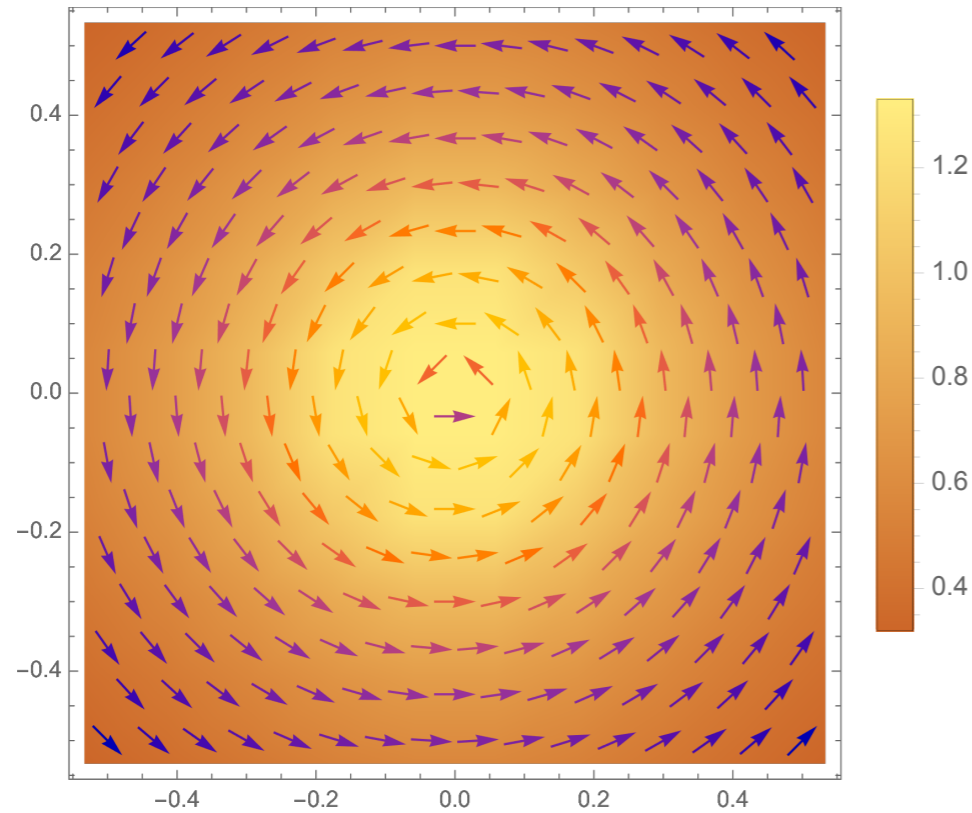
Electromotive force  $V_H$  is induced in the direction perpendicular to both the electric current and magnetic field

(In metal,  $V_H$  is too small to observe)

b). Anomalous quantum Hall effect

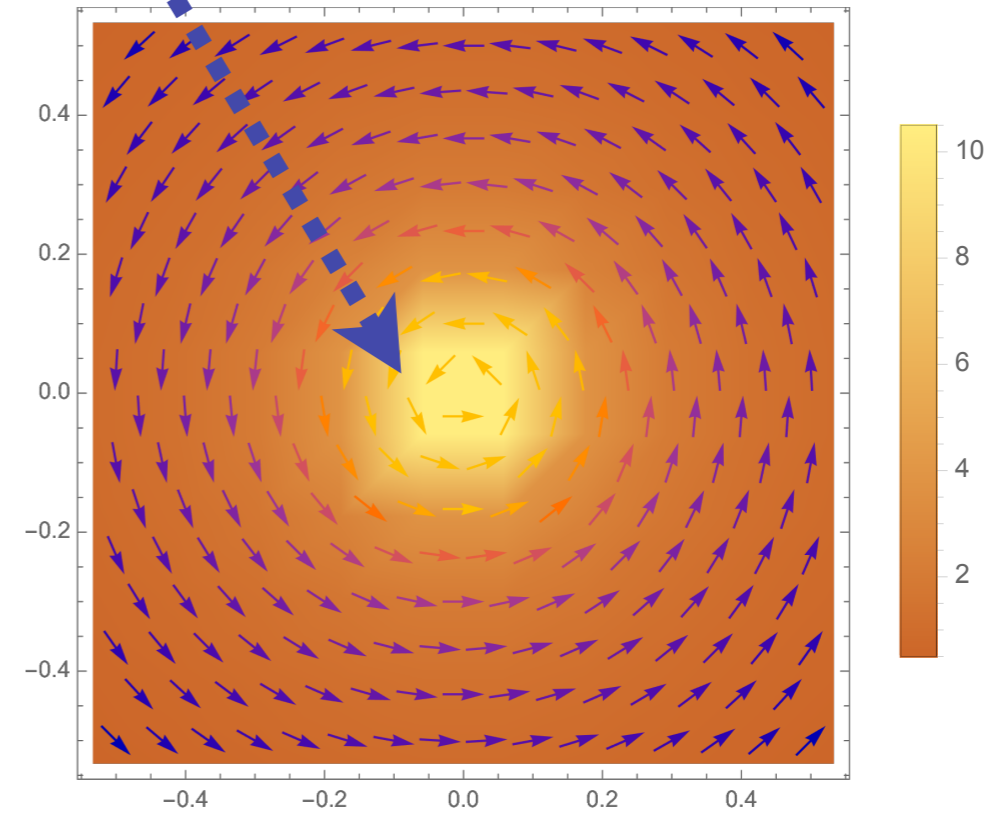
$a(k)$

$m = 0.1$



Singular at  $k = 0$

$m = -0.1$

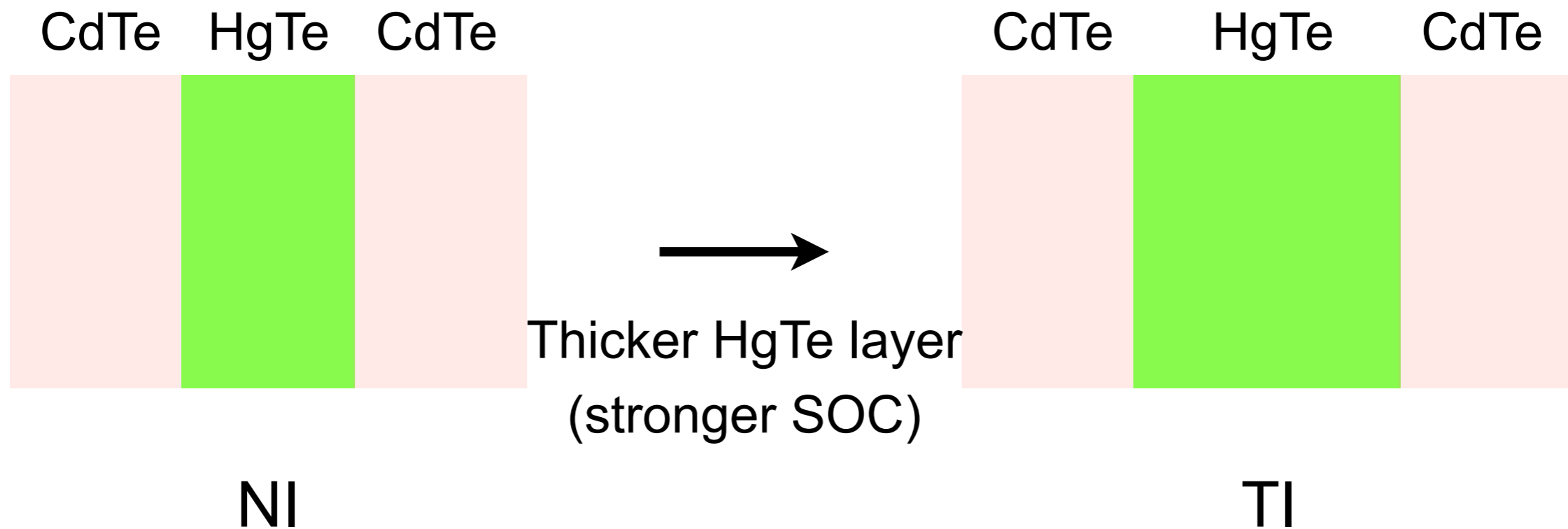


→ Integer  $\nu$

Note:  $\nu$  is half-integer if the dispersion relation is Dirac type

# Example of 2D TI: HgTe/(Hg, Cd)

König et al. '07

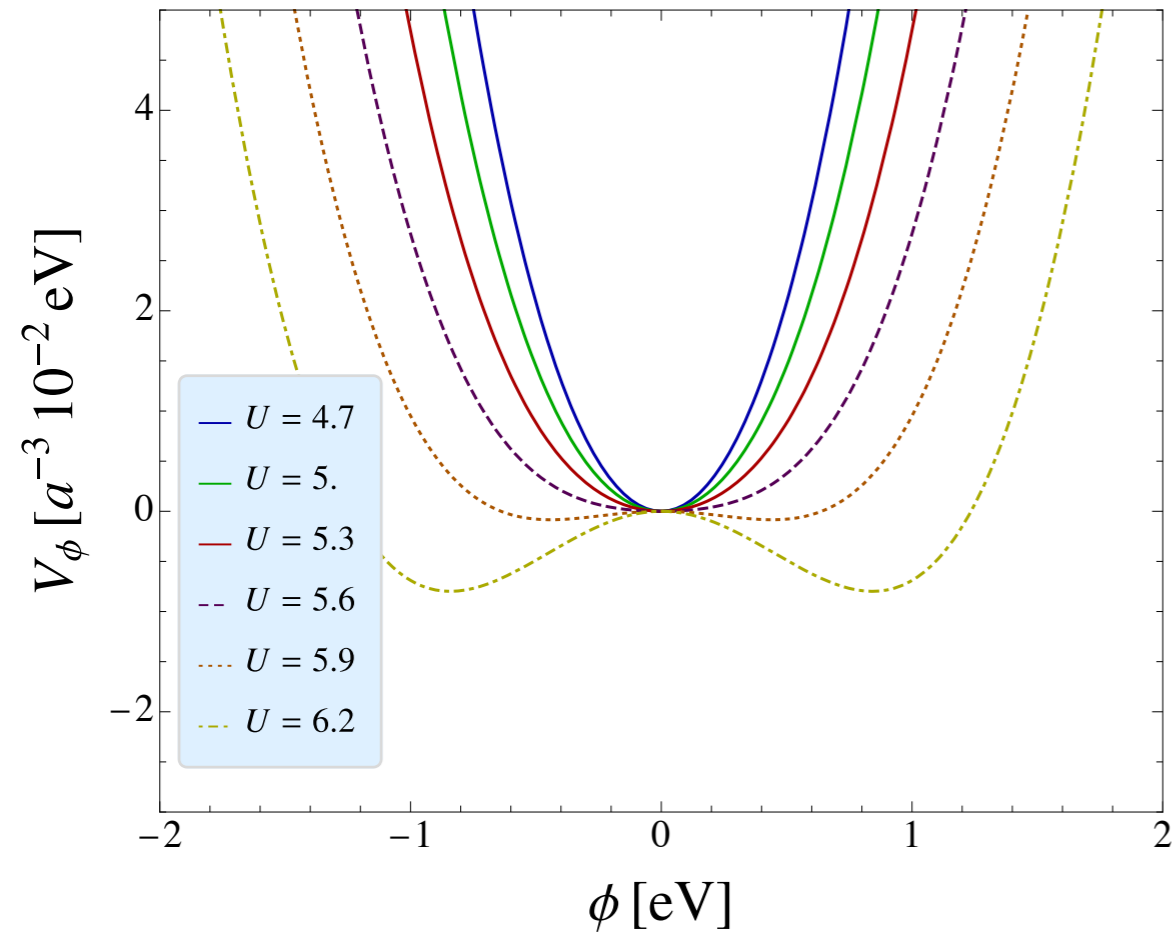


Band inversion happens in the energy band of HgTe

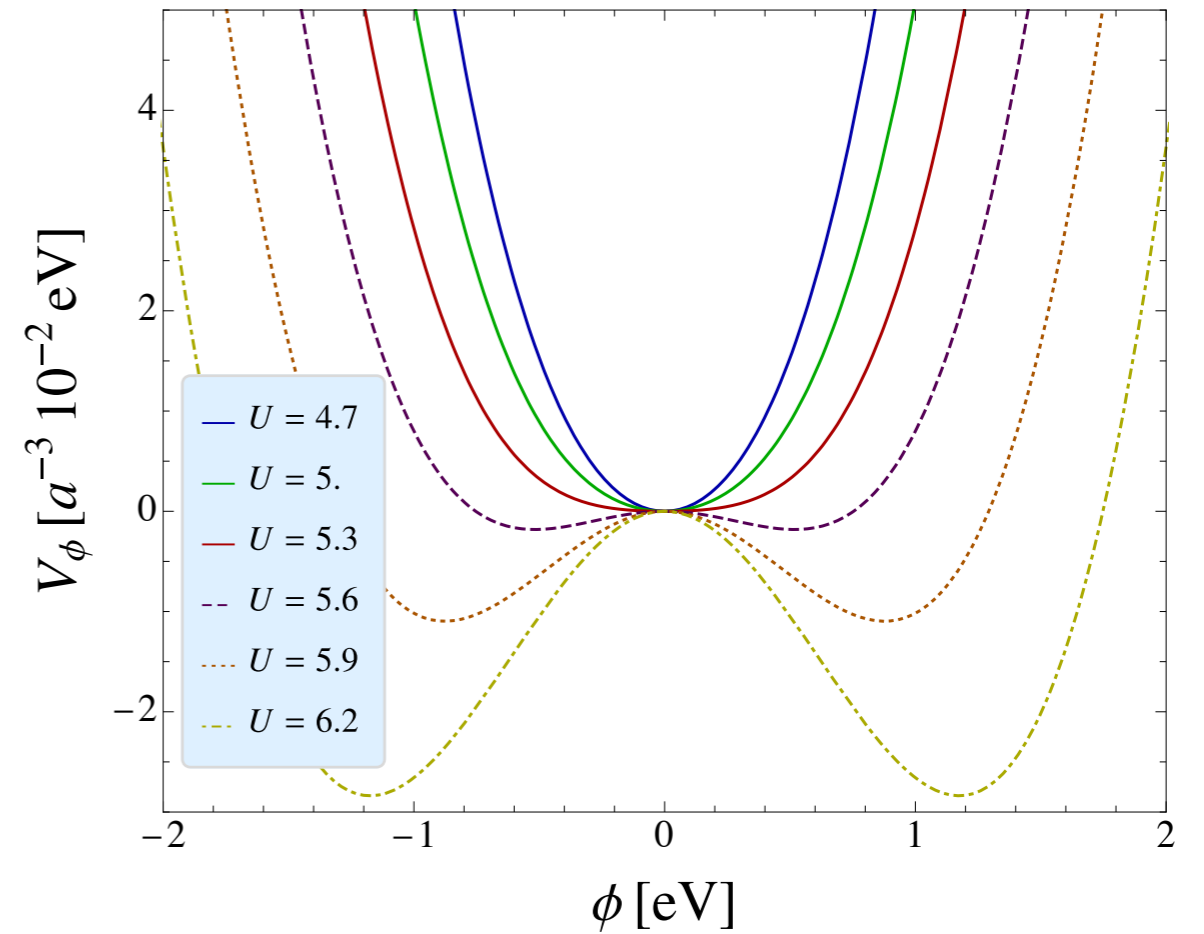
# $M$ dependence

KI '21

Effective model for 3D TI,  $M$  [eV] = 0.1

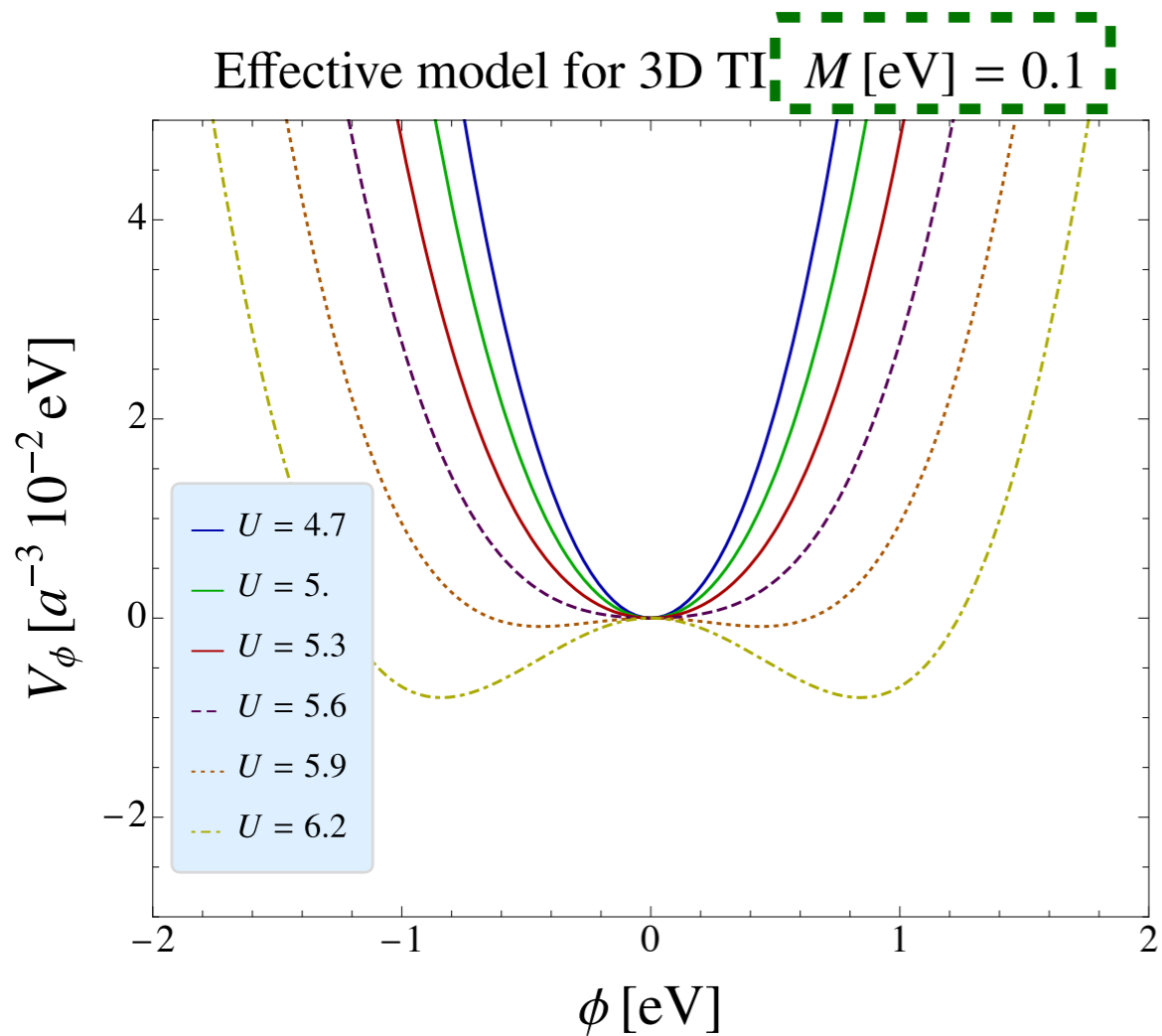


Effective model for 3D TI,  $M$  [eV] = -0.1

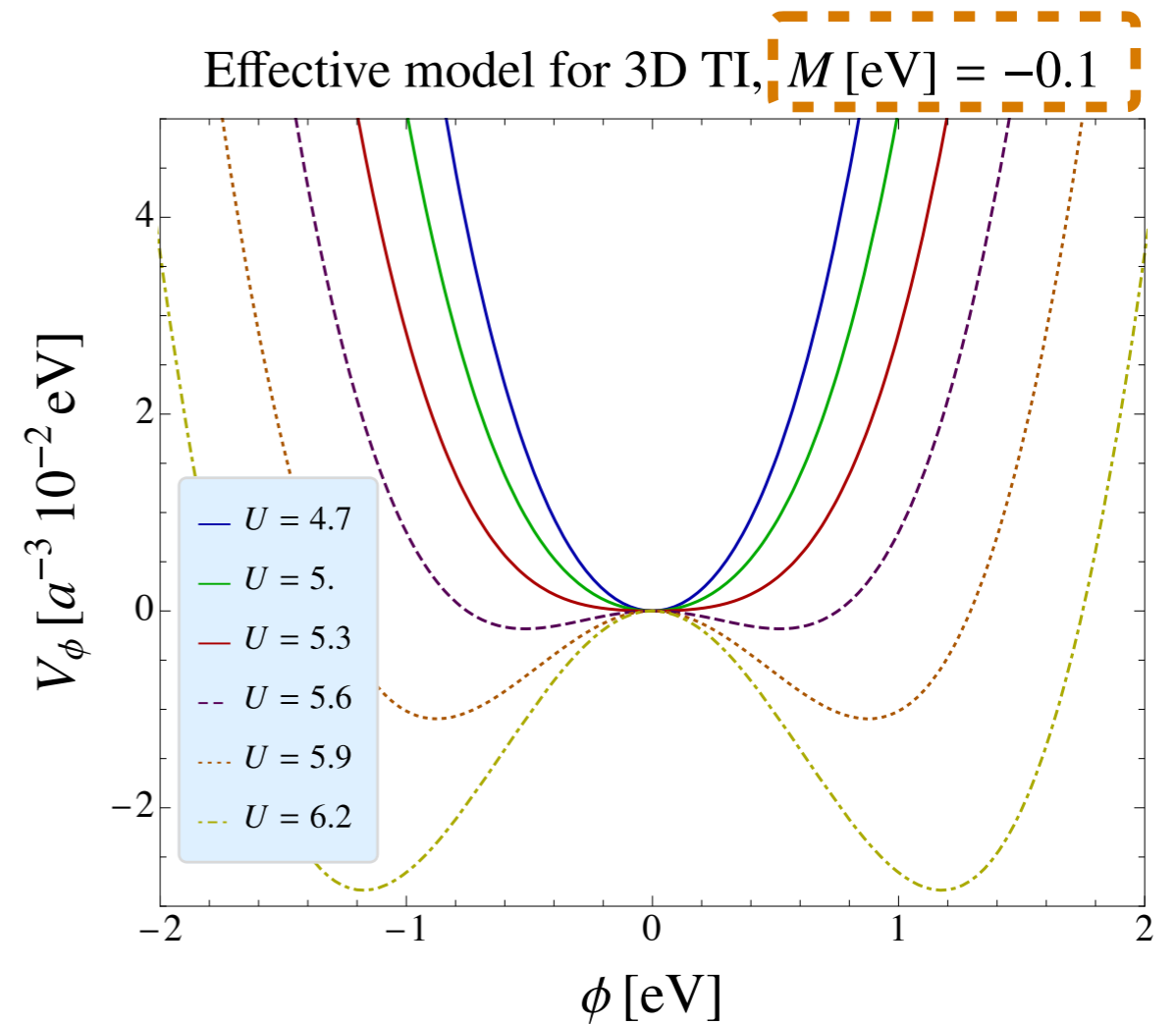


# M dependence

KI '21



NI



TI

The difference between TI and NI is not clear

Recall ME effect in TI is described by

$$\mathcal{L}_\theta = -\frac{\alpha}{4\pi} \int d^4x \theta F_{\mu\nu} \tilde{F}^{\mu\nu} \quad \text{with} \quad \theta = \pm\pi$$

- $\theta = \pm\pi$  for TI
- $\theta = 0$  for NI

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$\theta$  is the order parameter of phase transition between TI and NI

We need potential for  $\theta$

$\theta$  can be computed from Hamiltonian:

- $$\theta = \frac{1}{4\pi} \int d^3k \frac{2|d| + d^4}{(|d| + d^4)^2 |d|^3} \epsilon^{ijkl} d^i \partial_{k_x} d^j \partial_{k_y} d^k \partial_{k_z} d^l$$

R. Li et al. '10

- Approximately given by chiral anomaly (Fujikawa method)



## Derivation as chiral anomaly

$$H(\mathbf{k}) = \sum_{a=1}^5 d^a(\mathbf{k}) \Gamma^a$$

$$(d^1, d^2, d^3, d^4, d^5) = (A_2 \sin k_x, A_2 \sin k_y, A_1 \sin k_z, \mathcal{M}(\mathbf{k}), \phi)$$

$$\mathcal{M}(\mathbf{k}) = M - 2B_1 - 4B_2 + 2B_1 \cos k_z + 2B_2(\cos k_x + \cos k_y)$$

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- expand around  $\mathbf{k} = 0$
- redefine  $\mathbf{k}$

$$H(\mathbf{k}) = k_x \Gamma^1 + k_y \Gamma^2 + k_y \Gamma^3 + M \Gamma^4 + \phi \Gamma^5$$

“Dirac model”

$$H(\mathbf{k}) = k_x \Gamma^1 + k_y \Gamma^2 + k_y \Gamma^3 + M \Gamma^4 + \phi \Gamma^5$$



Unitary transformation of the basis

$$\tilde{U} H(\mathbf{k}) \tilde{U}^\dagger = \beta(\boldsymbol{\gamma} \cdot \mathbf{k} + M + \phi \gamma_5)$$

.....→

$$S = \int d^4x \bar{\psi} [i\gamma^\mu (\partial_\mu - ieA_\mu) - M - i\phi\gamma_5] \psi$$

$\Gamma^5 \phi$  reduces to  $i\gamma^5 \phi$

$i\gamma^5\phi$  term can be rotated away, which gives rise to  $\theta$  term:

$$S_{\Theta} = -\frac{\alpha}{4\pi} \int d^4x \Theta F_{\mu\nu} \tilde{F}^{\mu\nu}$$

$$\Theta = \frac{\pi}{2} [1 - \text{sgn}(M)] \text{sgn}(\phi) + \tan^{-1} \frac{\phi}{M}$$

it is consistent with

$$\theta = \frac{1}{4\pi} \int d^3k \frac{2|d| + d^4}{(|d| + d^4)^2 |d|^3} \epsilon^{ijkl} d^i \partial_{k_x} d^j \partial_{k_y} d^k \partial_{k_z} d^l$$

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$$\phi = \phi(\theta)$$

$$V_{\phi}(\phi)$$

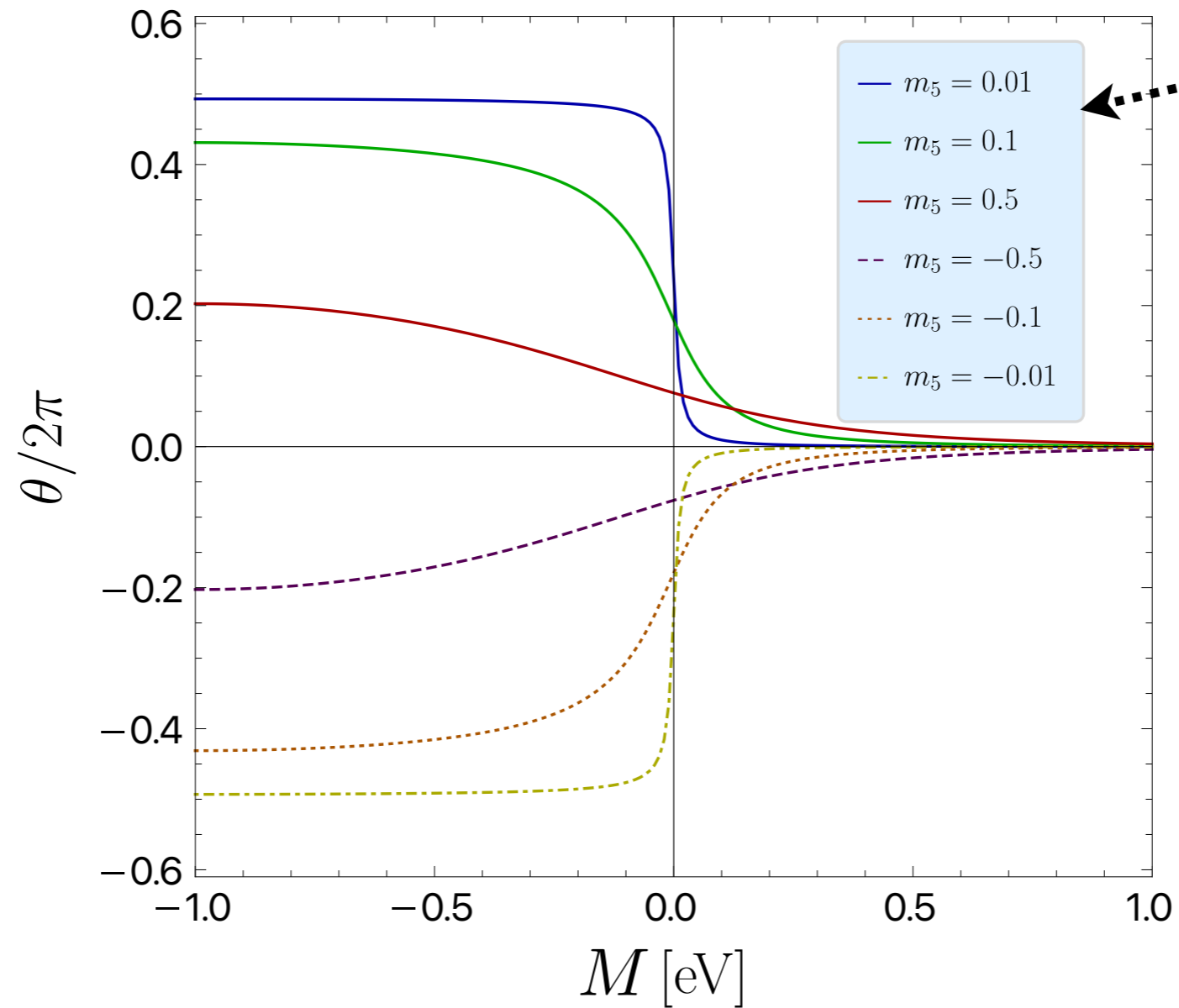


$$V_{\theta}(\theta)$$

# $\theta$ as function of $M$

KI '21

Effective model for 3D TI

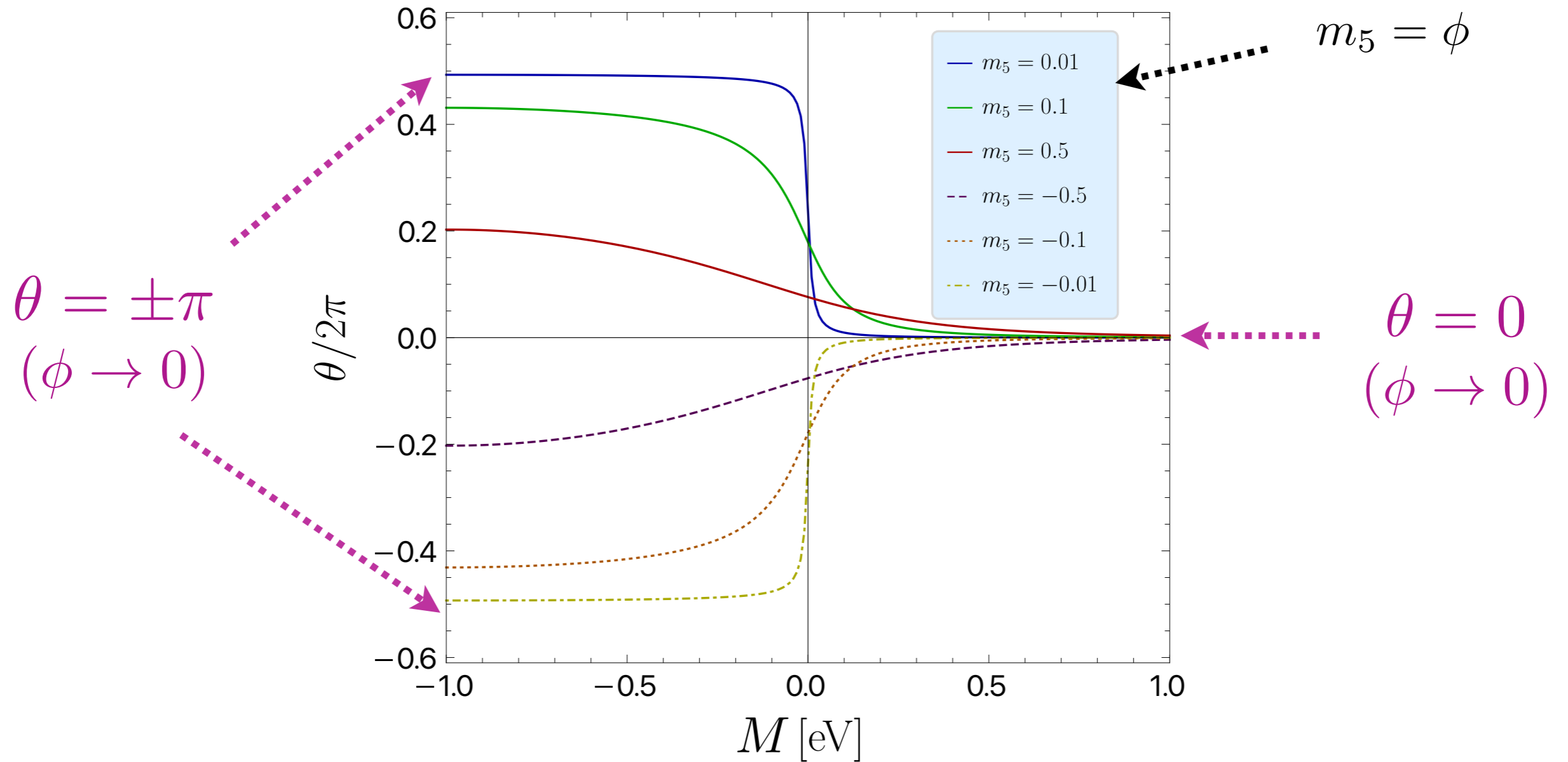


calculation for Dirac  
model is done by  
Zhang '19

# $\theta$ as function of $M$

KI '21

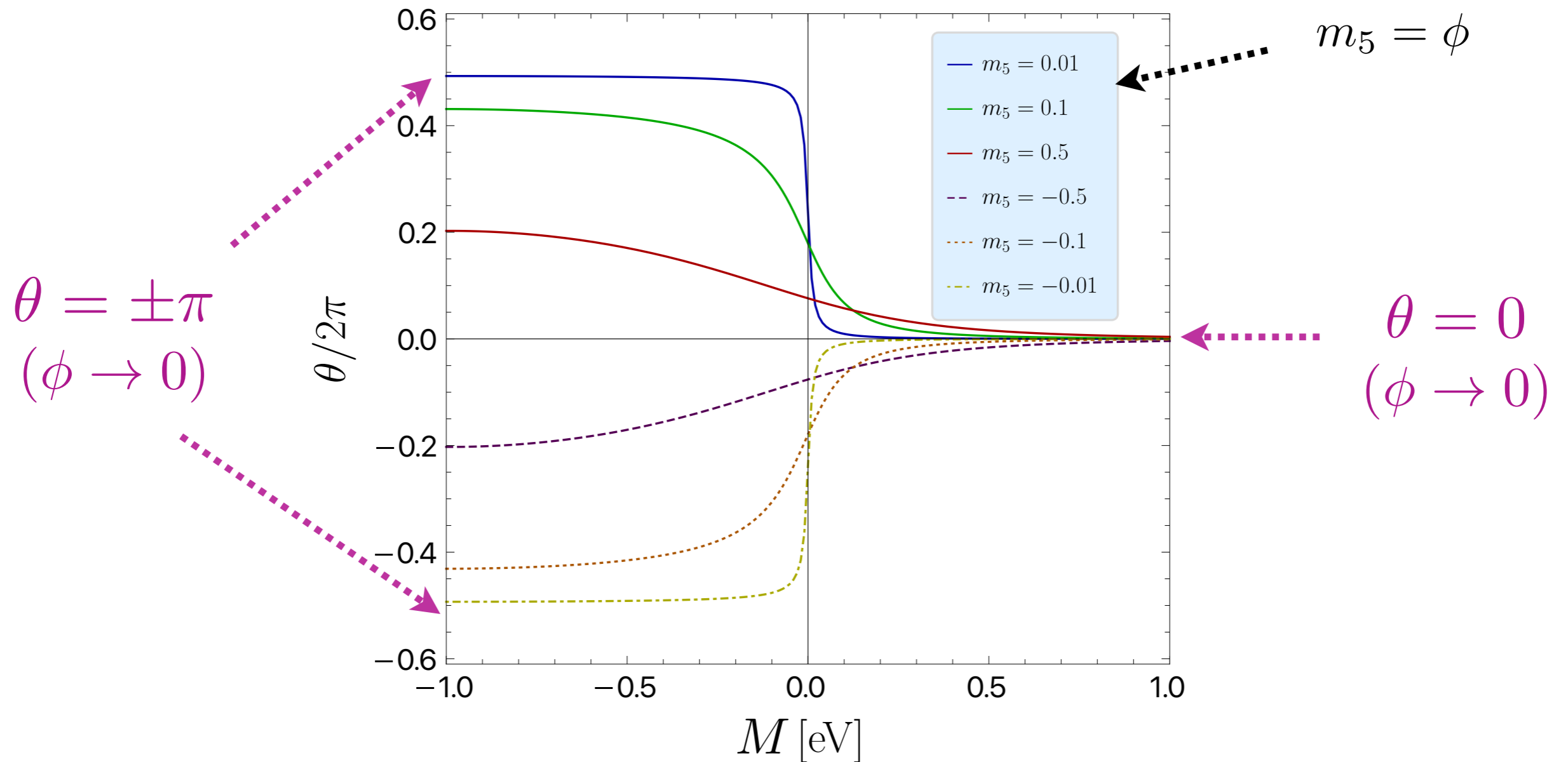
Effective model for 3D TI



# $\theta$ as function of $M$

KI '21

Effective model for 3D TI



$\phi = 0$   
( $\mathcal{T}$ )  $\longleftrightarrow$  PM order



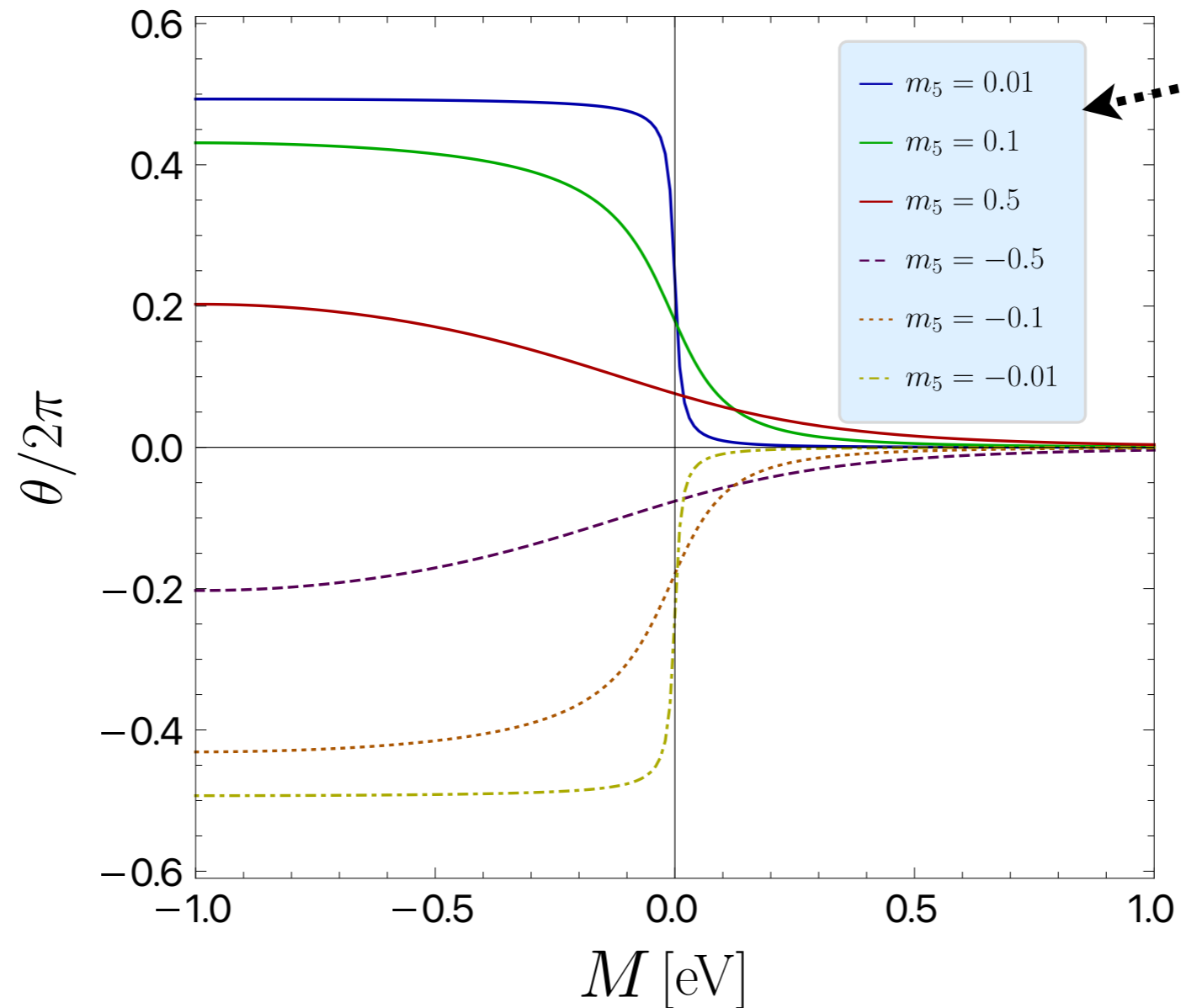
$\theta = \pm\pi$      $M < 0$     (TI)  
 $\theta = 0$          $M > 0$     (NI)



# $\theta$ as function of $M$

KI '21

Effective model for 3D TI



$m_5 = \phi$

$\phi \neq 0$   
( ~~$\mathcal{F}$~~ )  $\longleftrightarrow$  AFM order



$\theta$  takes continuum variable

# $\theta$ as function of $\phi$

Effective model for 3D TI

