Axion in antiferromagnetic insulators

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Based on PRD 104, no.1, 016004

Chiba, March 7, 2022

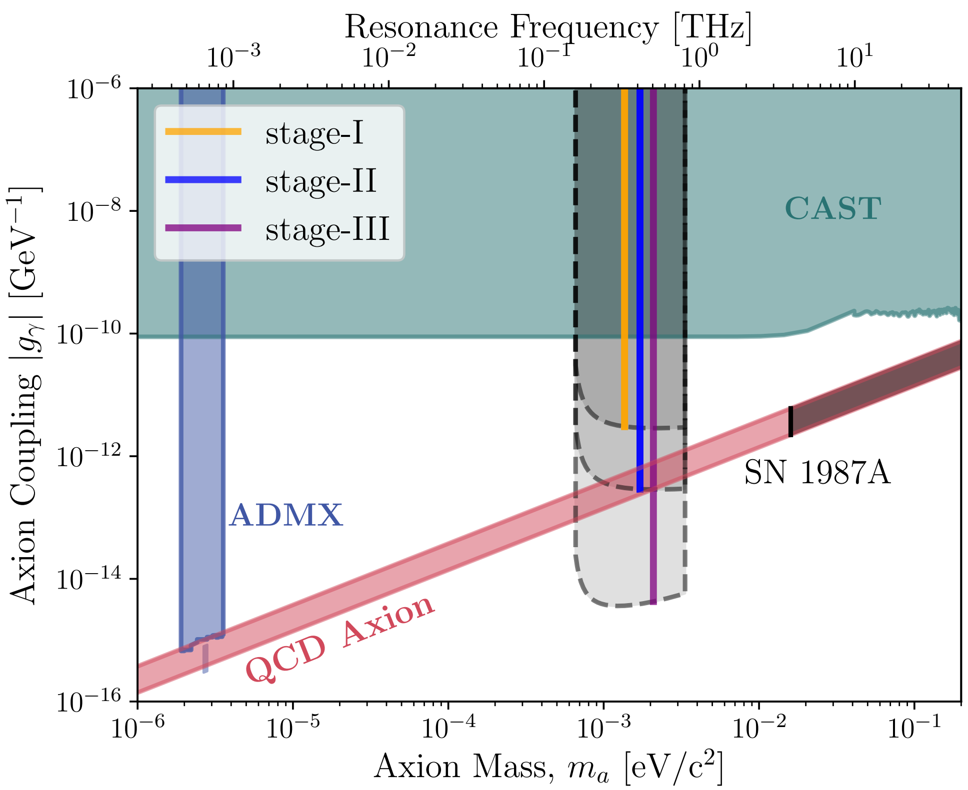
1. Introduction

Axion in condensed matter physics

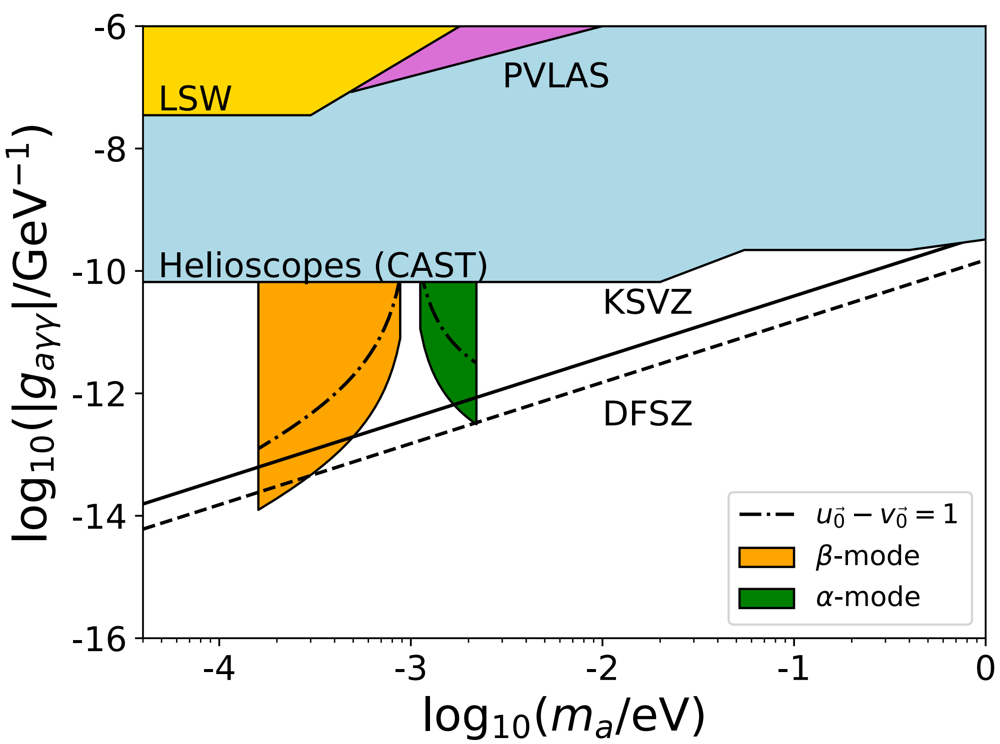
A hot topic and relates to

- Topological insulator
- Magnetoelectric effect
- Ferromagnetism / Antiferromagnetism
- It may be used in *particle* axion detection

Proposals to detect axion/axion-like particles (ALPs)



Marsh et al. '19



Chigusa et al. '21

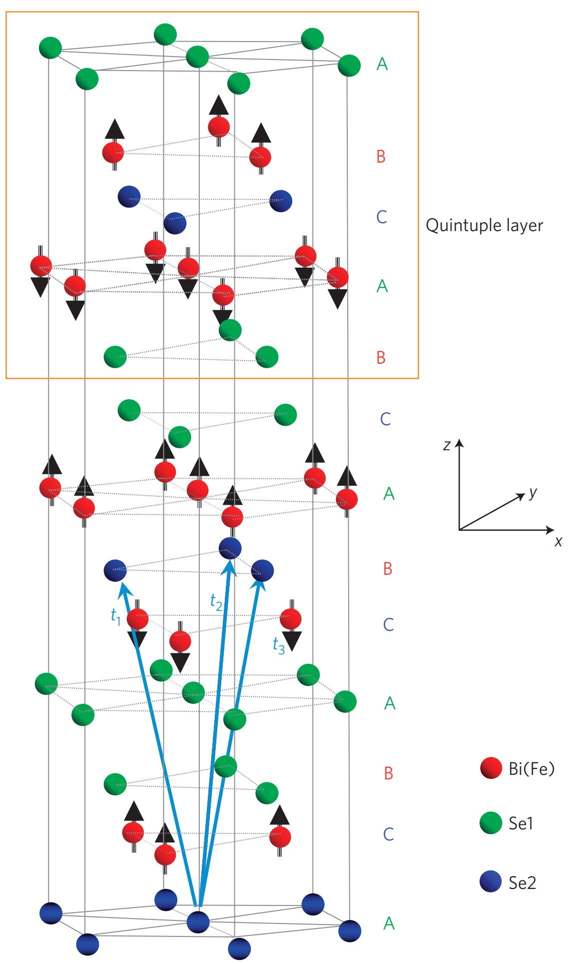
Topological magnetic insulators are used

Dynamical 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[1], Jing Wang[1,2], Xiao-Liang Qi[1] and Shou-Cheng Zhang[1]*



$\mathrm{Bi_2Se_3}$ ← Topological insulator

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

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

Axion mass ~ $\mathcal{O}(\mathrm{meV})$

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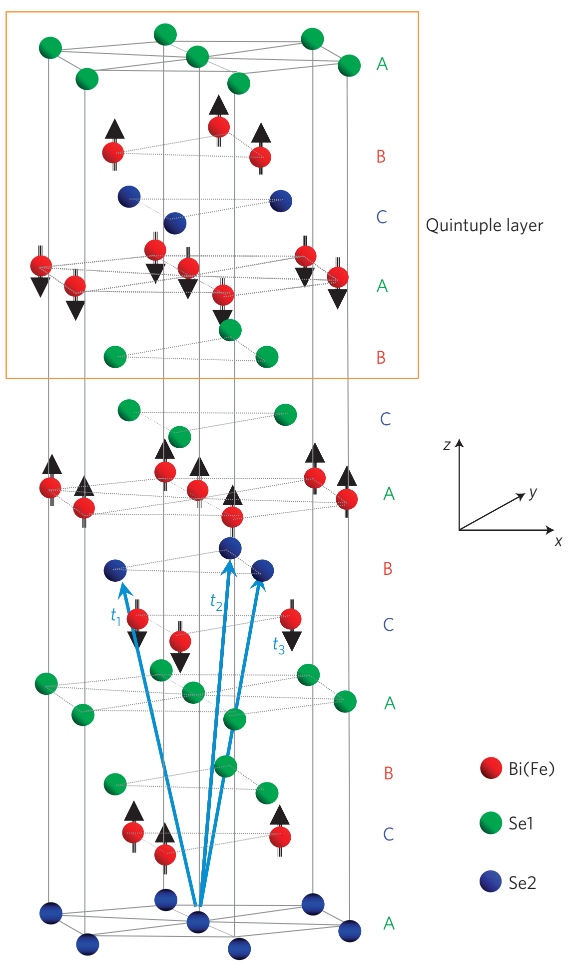
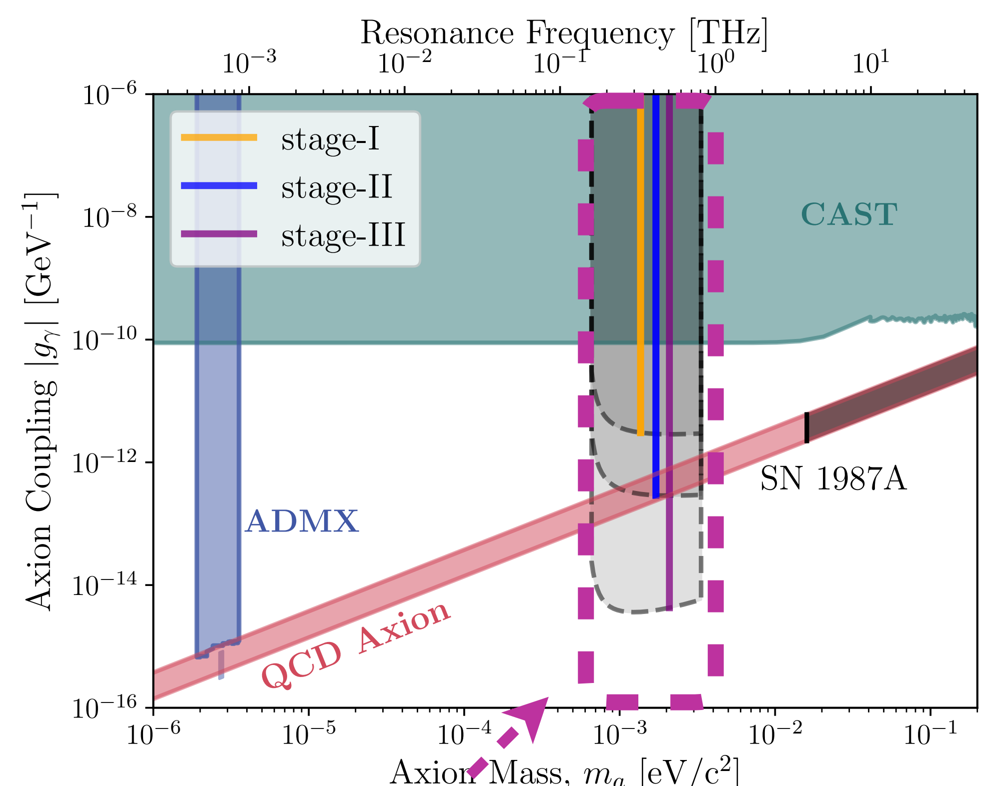




Marsh et al. '19

$\mathcal{O}(\mathrm{meV})$

Today, I would like to address

- What is topological insulator?
- How does antiferromagnetism 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

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

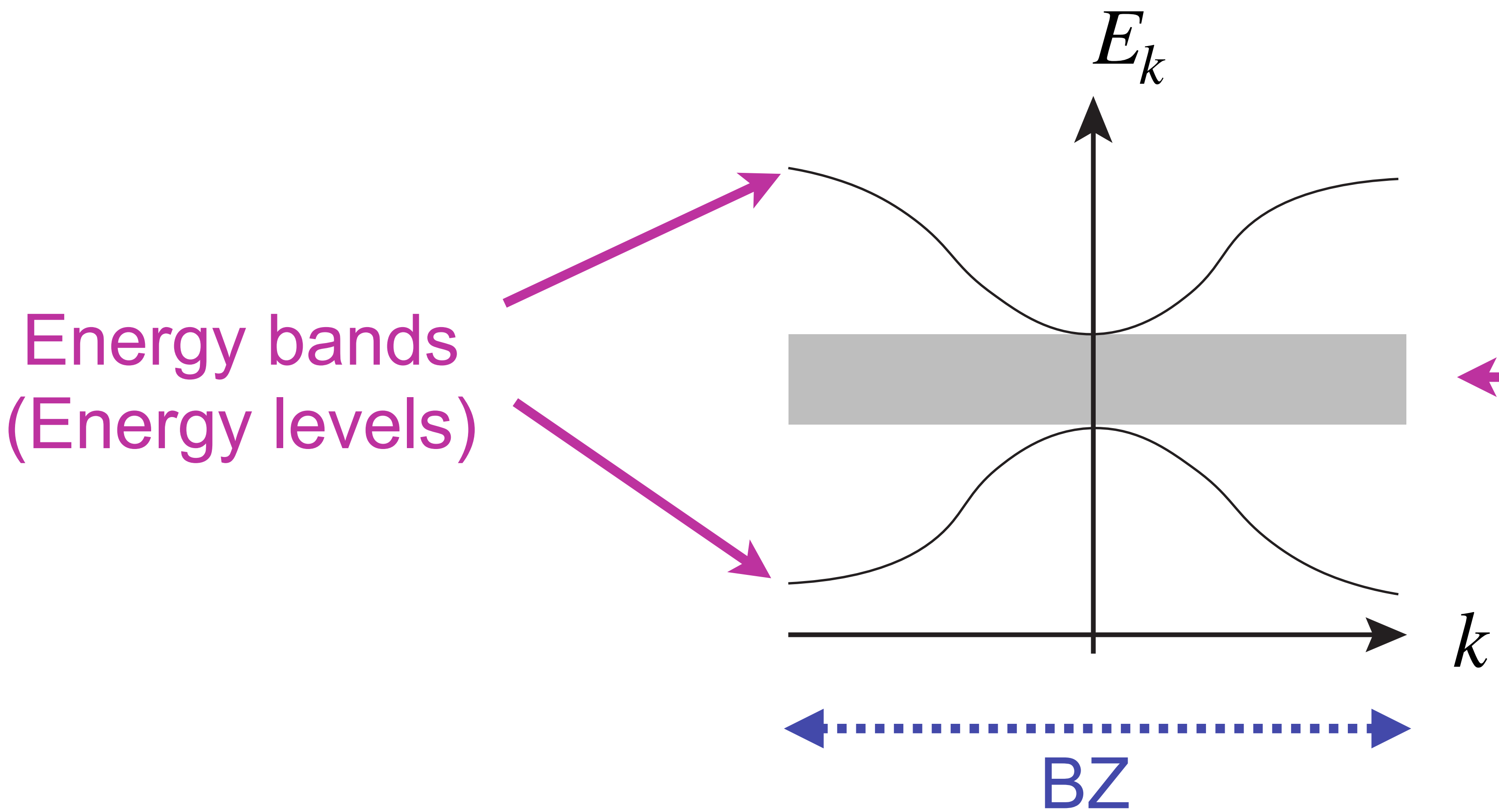
Topics related to axion in condensed matter physics

a). Insulators

b). Quantum Hall effect

c). Topological insulators

Minimum basics

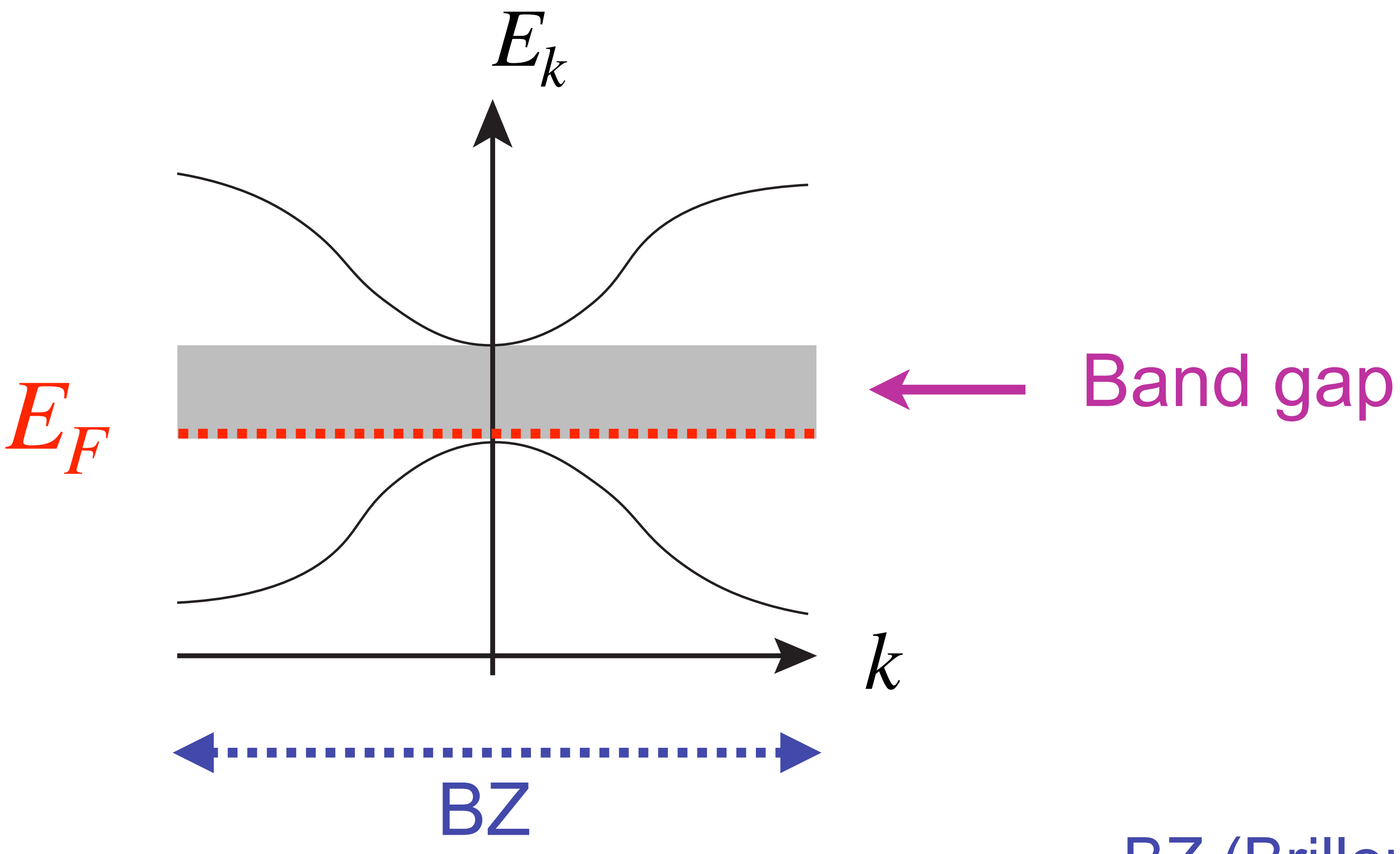


BZ (Brillouin zone)

E_k : energy of electron

k : wavenumber of electron

Minimum basics

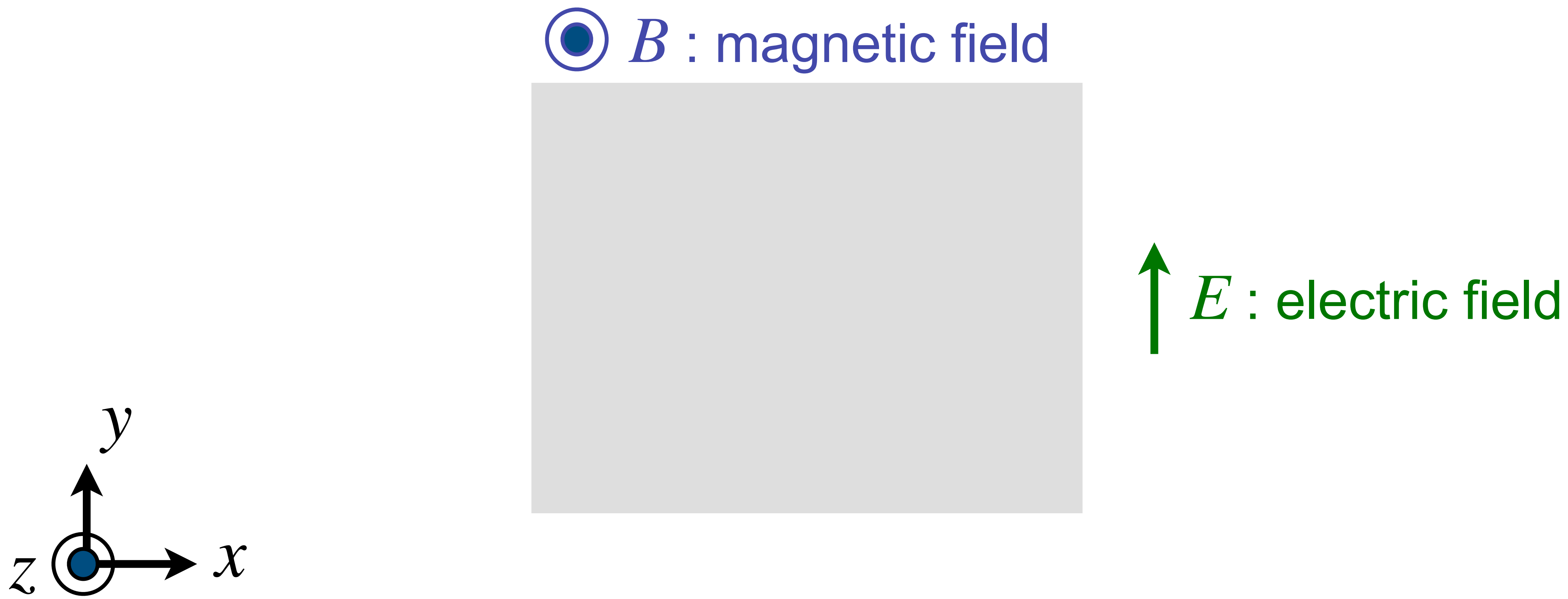


BZ (Brillouin zone)

→ Insulator

Quantum Hall (QH) effect

e.g., 2D insulator



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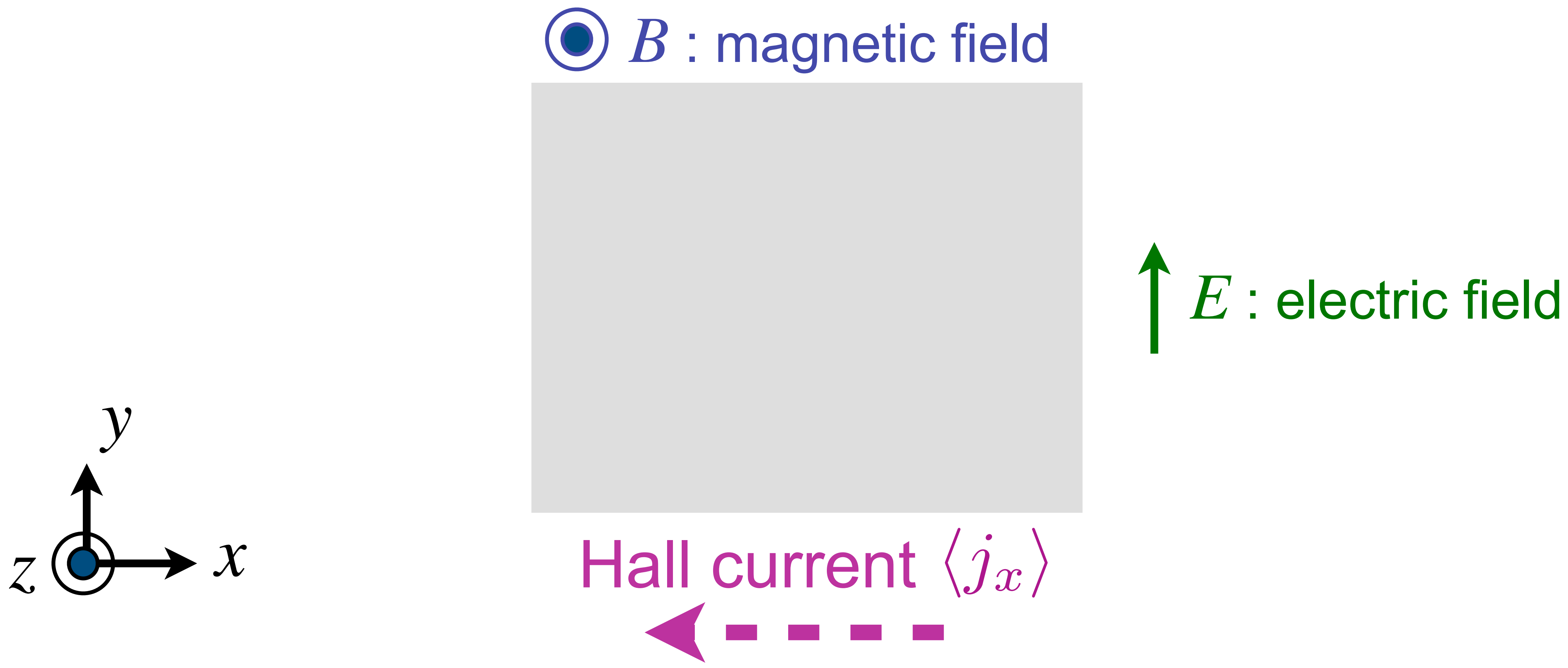
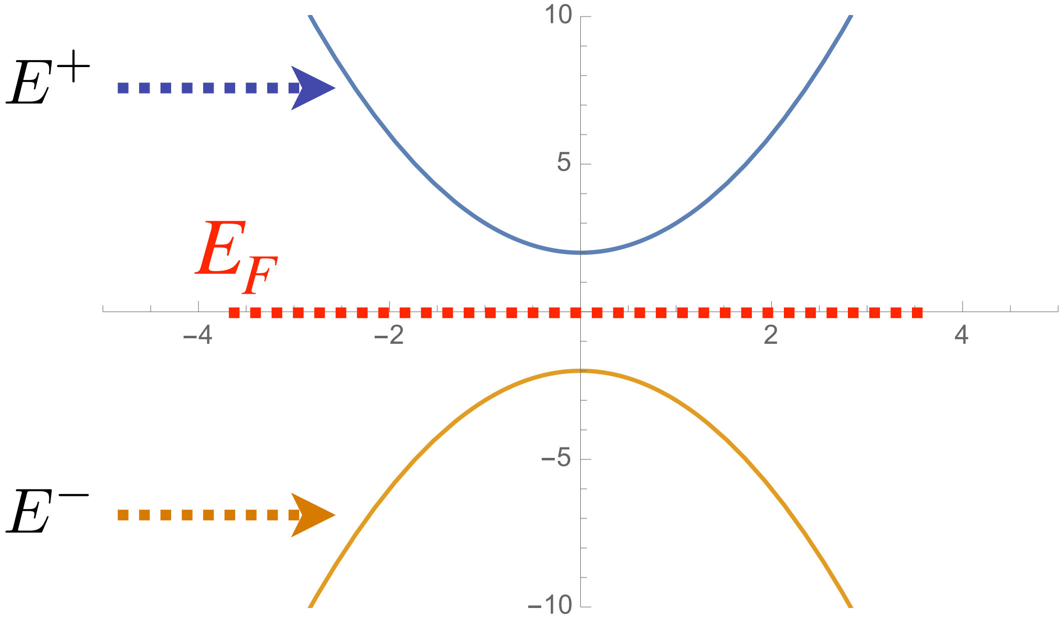


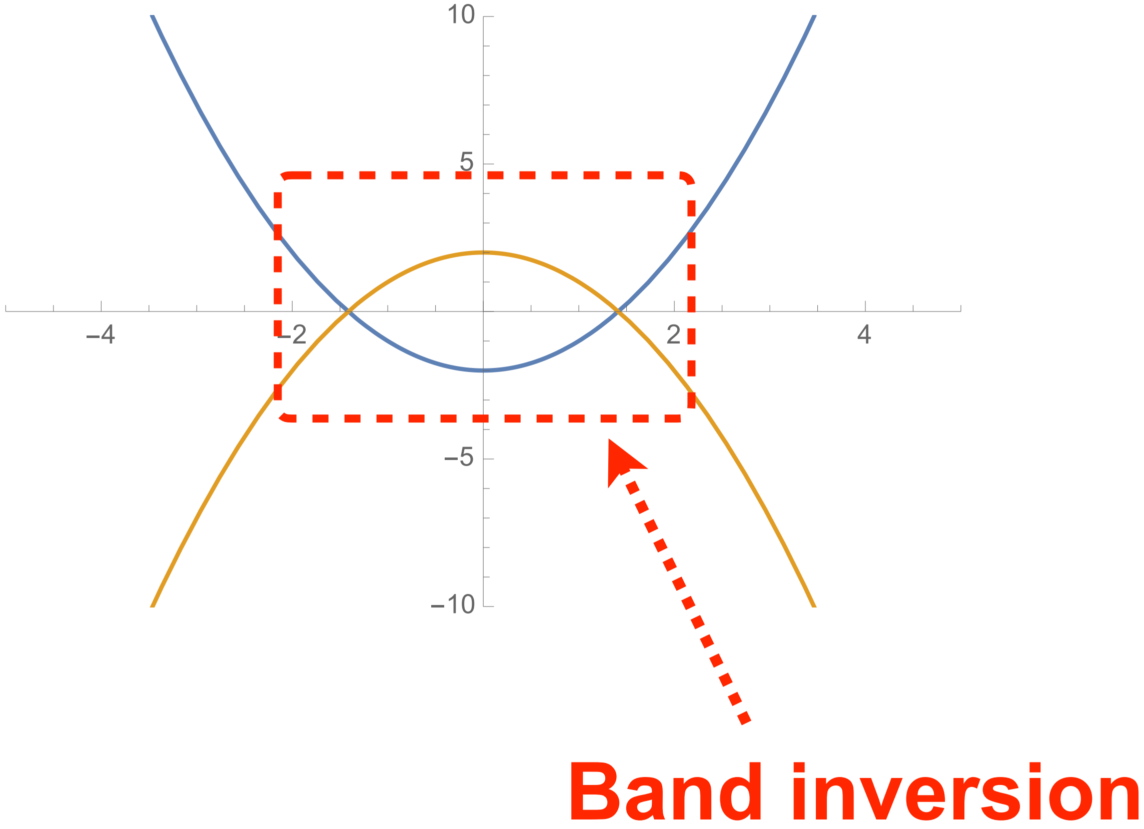
Quantized electric current is induced in x direction

"(Integer) QH effect"

The band structure



Normal insulator

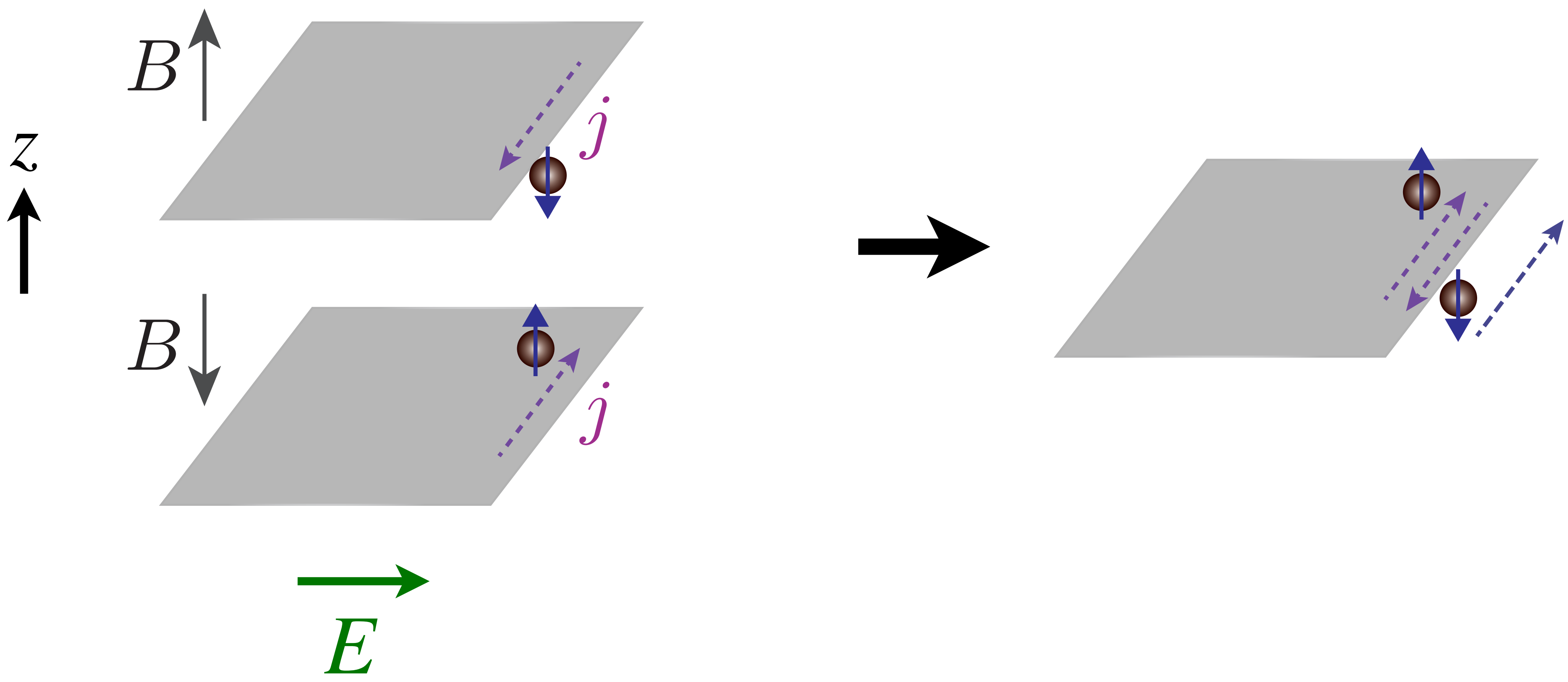


QH insulator

Topological insulators (TIs)

Kane, Mele ’05

Idea: combination of two QH insulators



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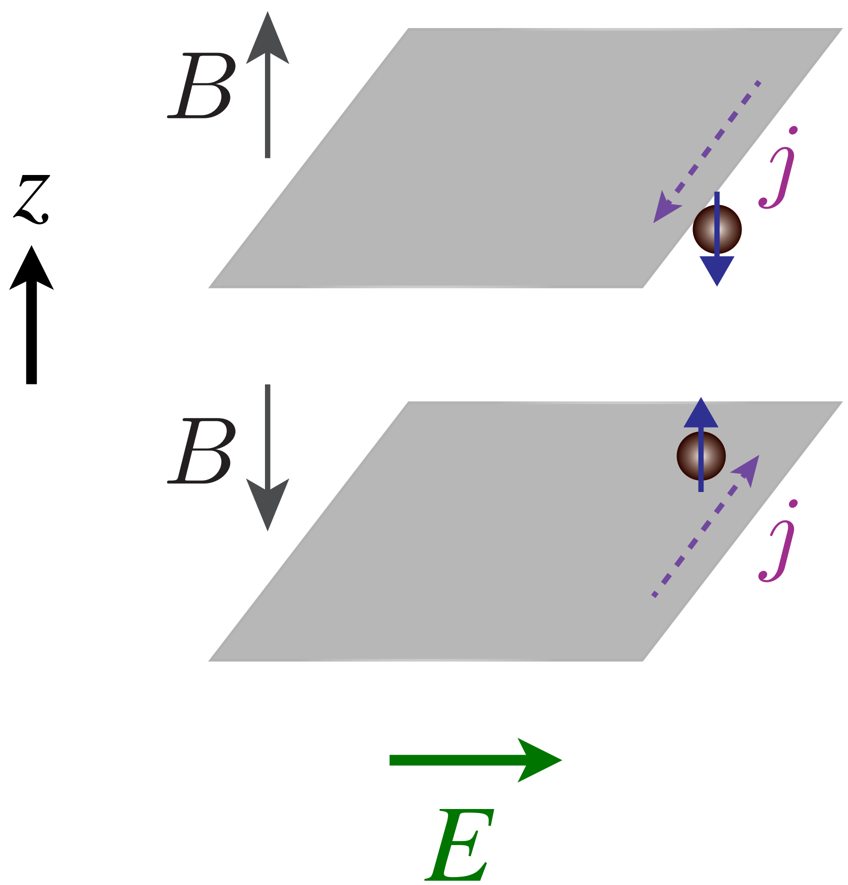

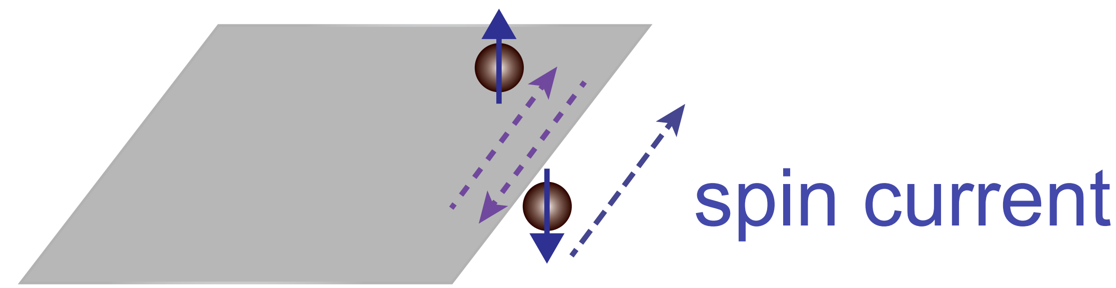

Hall current is zero, but
spin current exists

Topological insulators (TIs)

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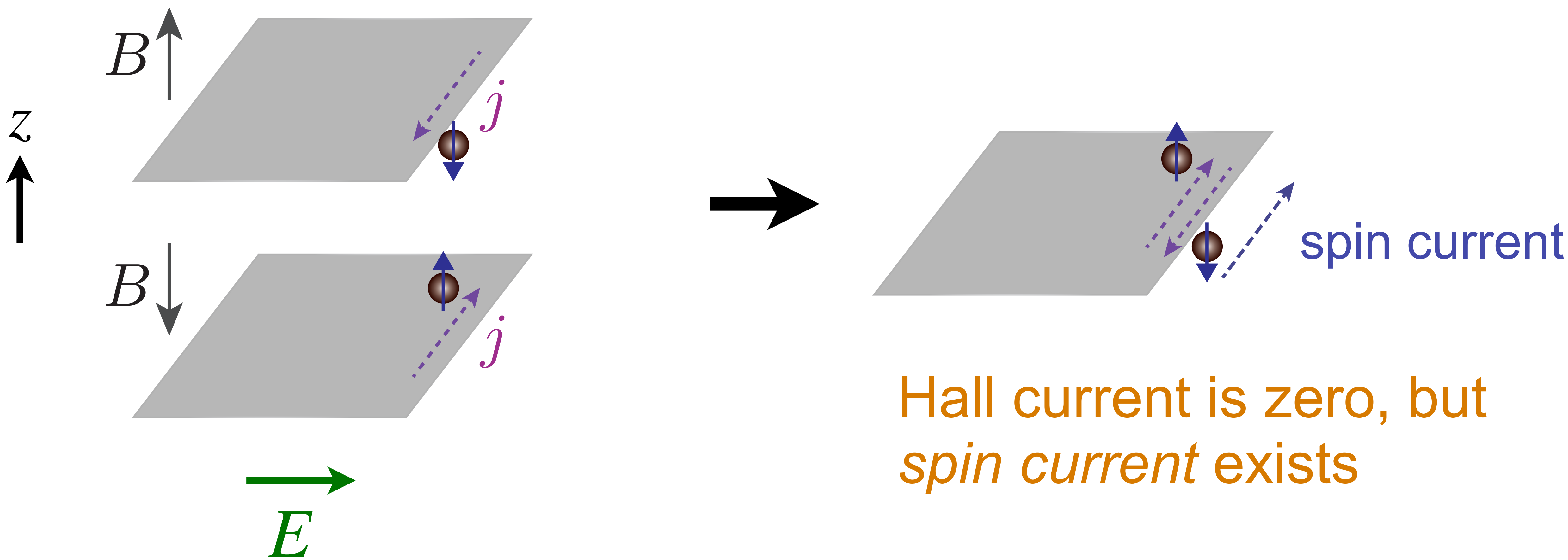


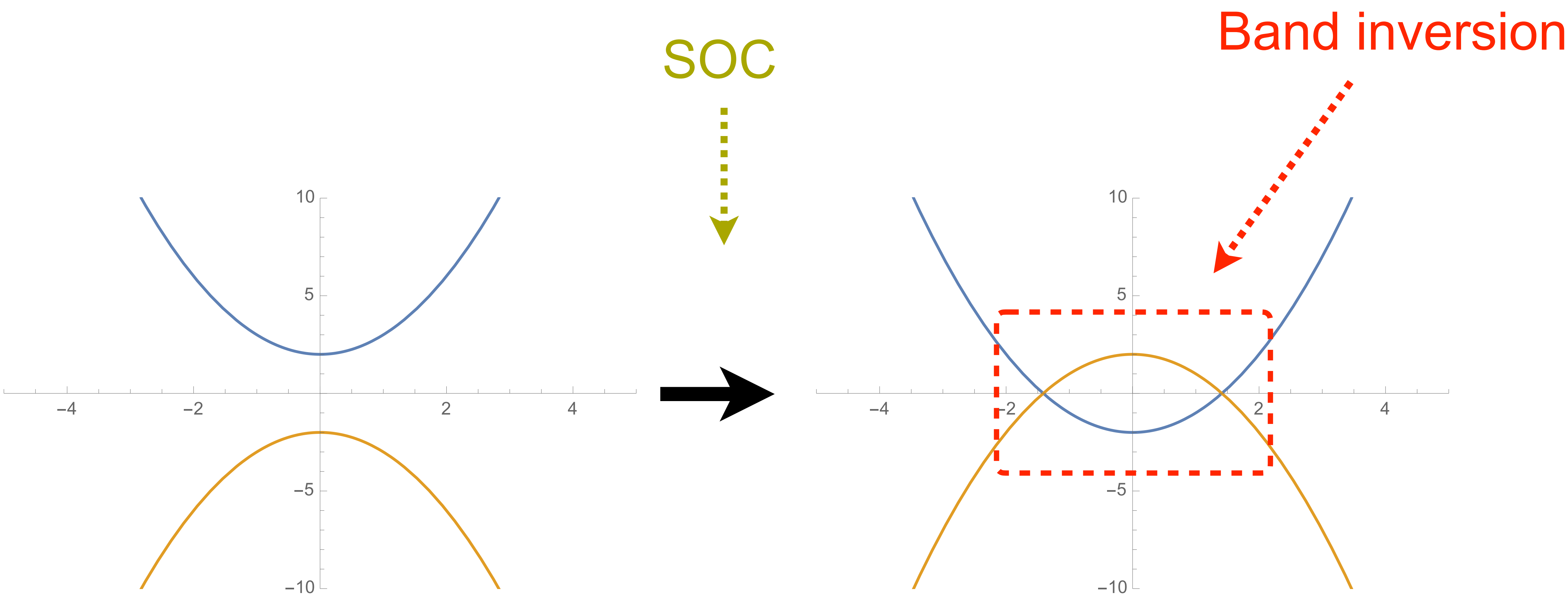
Hall current is zero, but *spin current* exists

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

SOC: spin orbit coupling

The band structure

→ The same as QH insulators



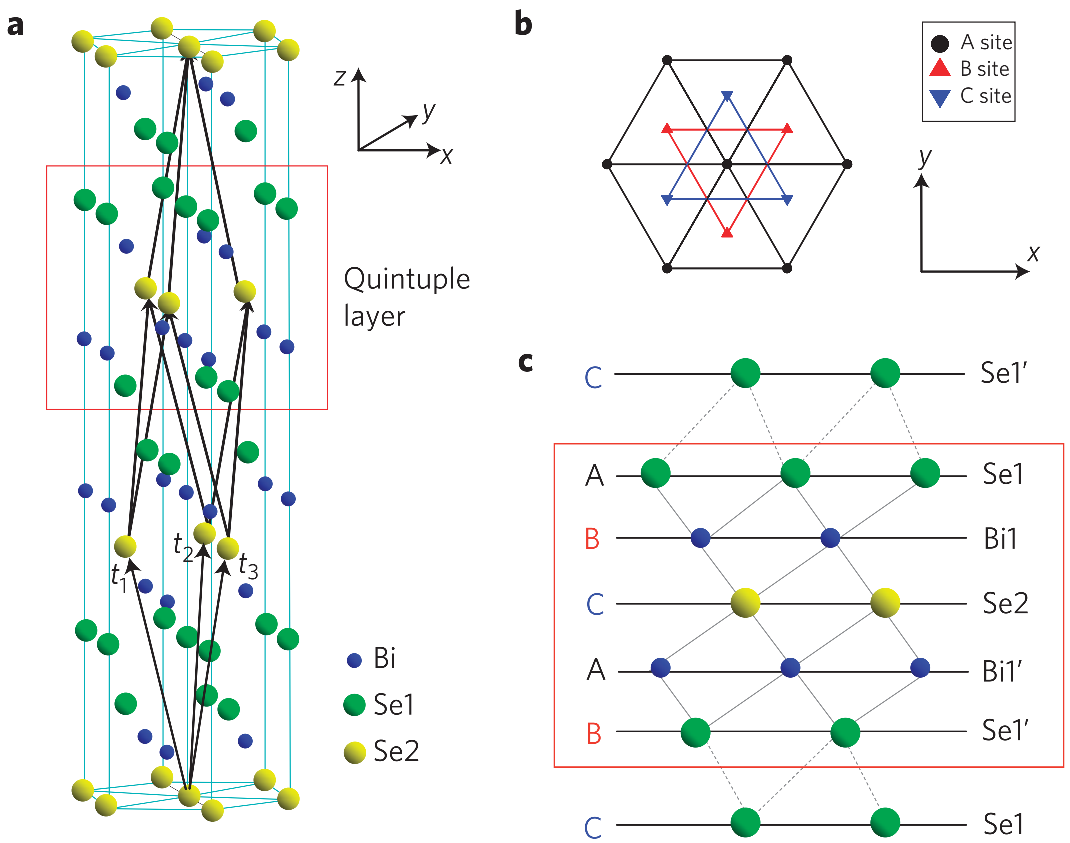
Normal insulator (NI)

Topological insulator (TI)

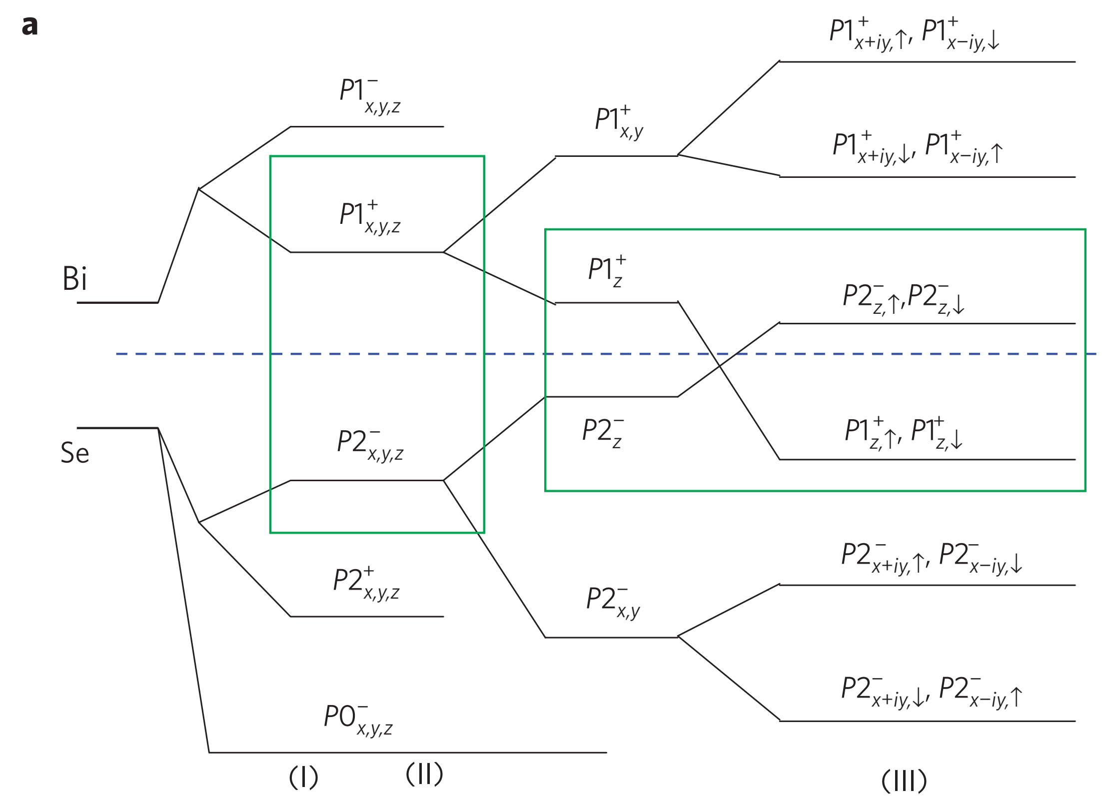
3. Axion in antiferromagnetic topological insulators

Let's consider 3D TI, Bi_2Se_3

H. Zhang et al. '09



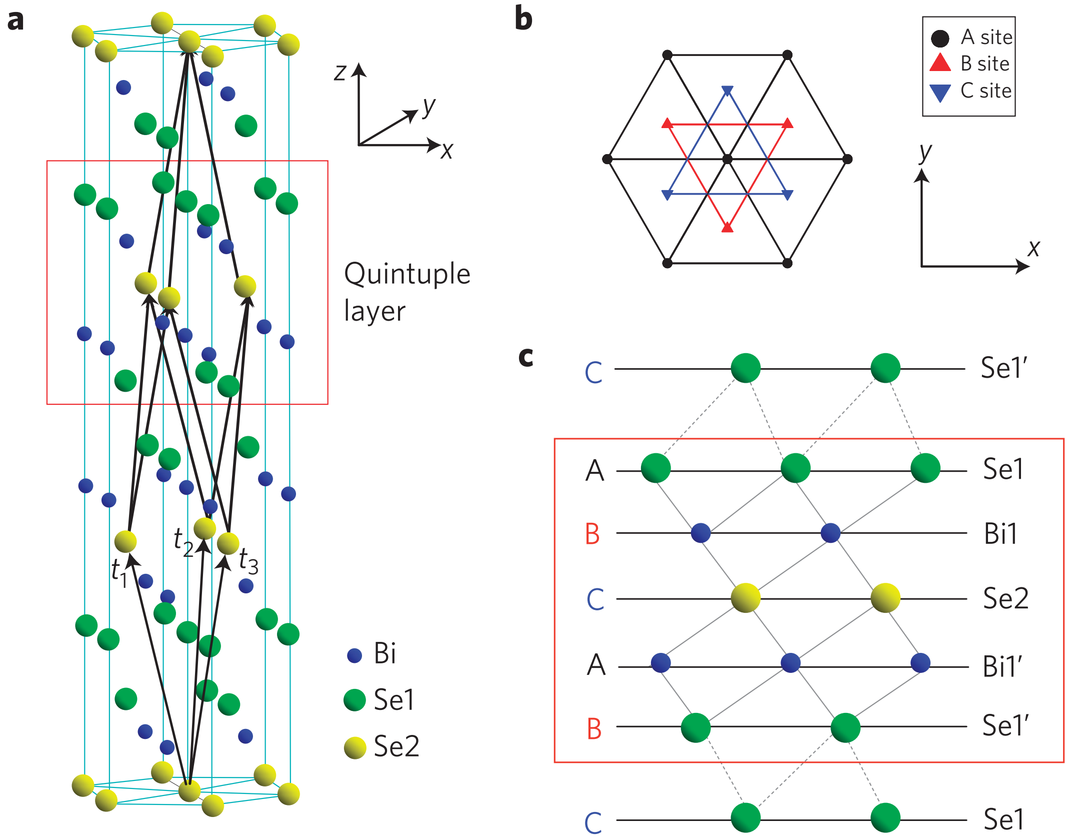
Cristal structure



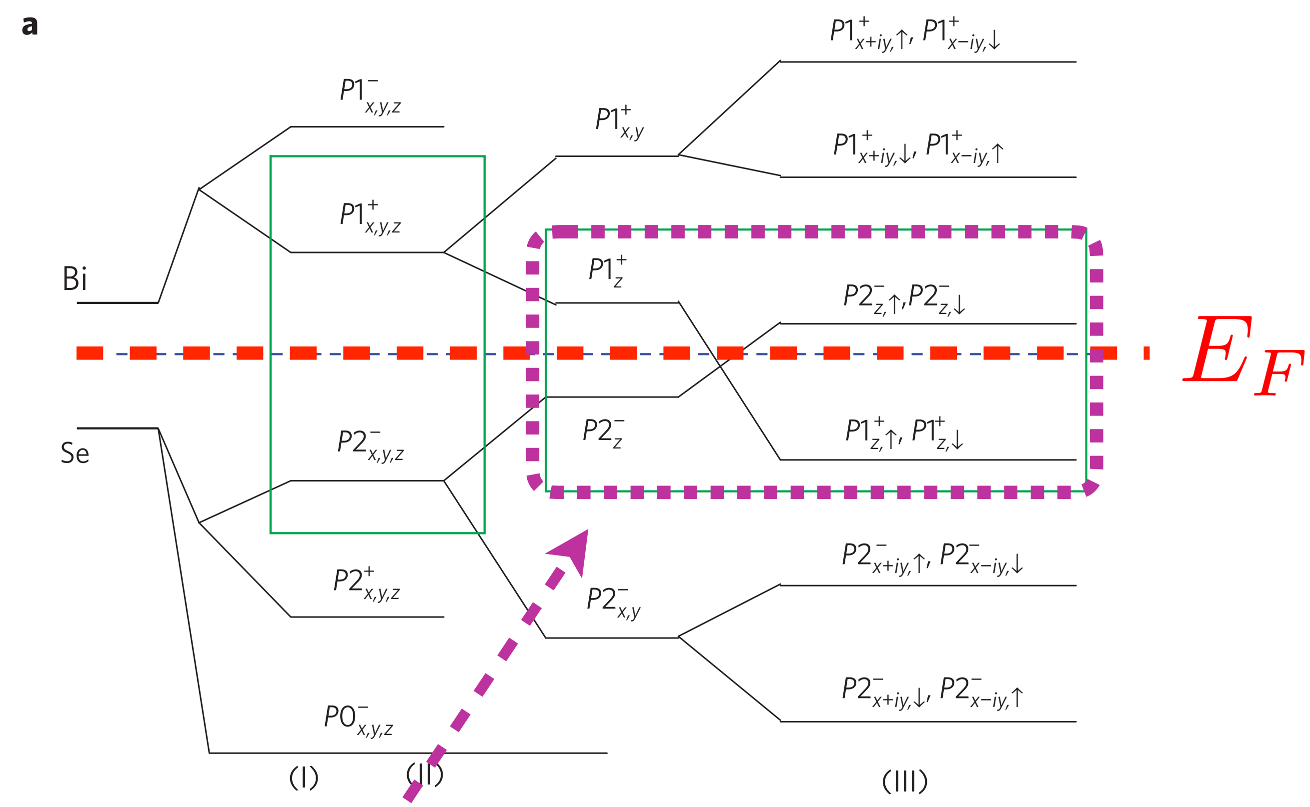
Energy levels

Let's consider 3D TI, Bi_2Se_3

H. Zhang et al. '09

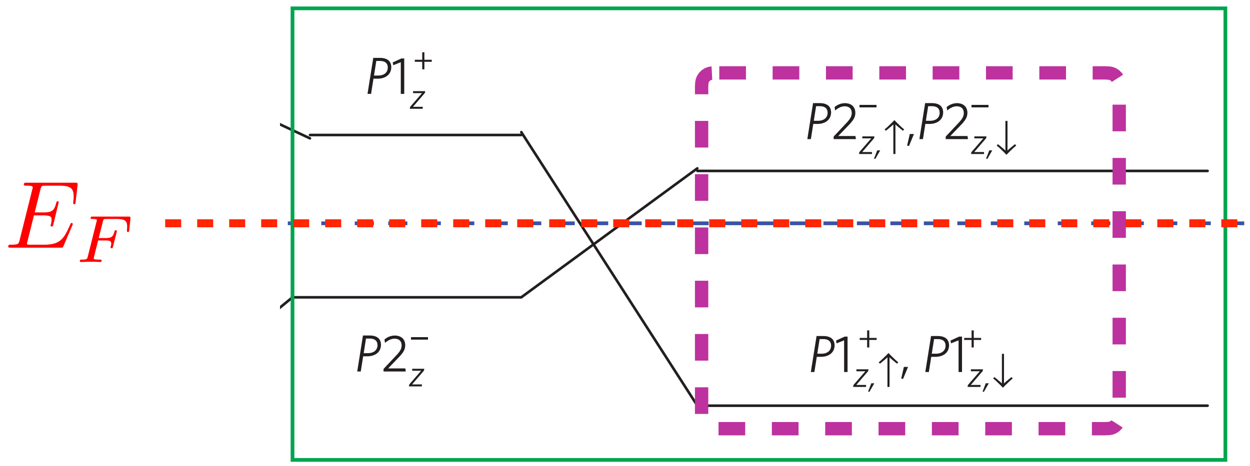


Cristal structure



Energy levels

Band inversion due to strong SOC



→ 4 by 4 matrices

$$H_0(\boldsymbol{k}) = \epsilon_0 \mathbf{1}_{4\times 4} + \sum_{a=1}^{5} d^a \Gamma^a$$

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

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

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

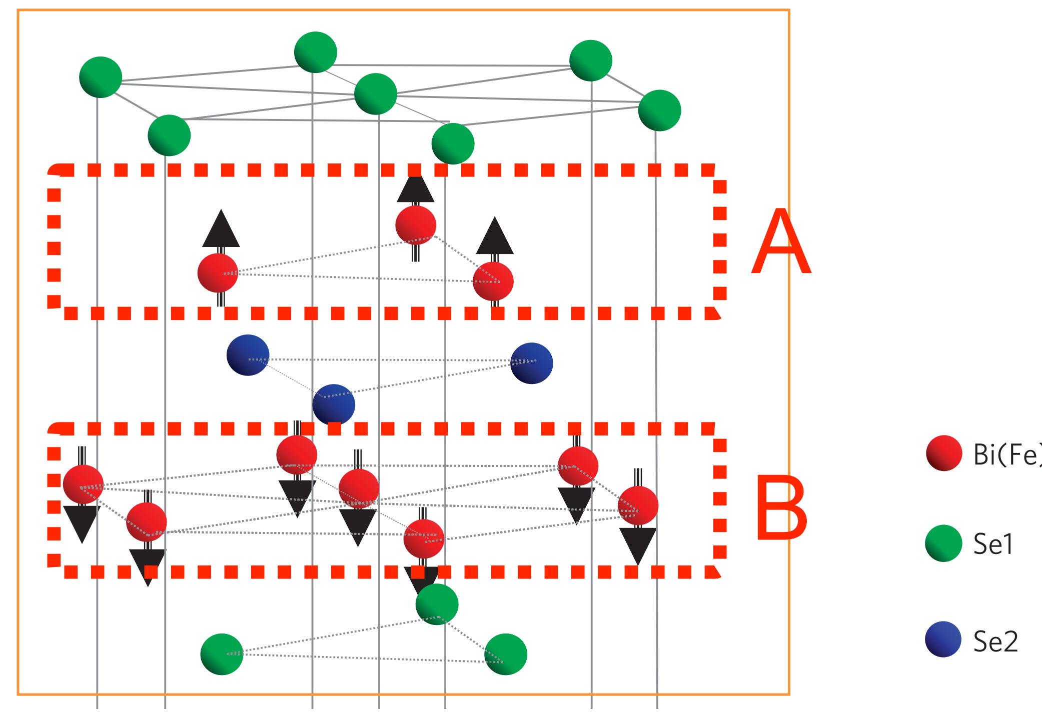
$$\Gamma^4 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad \Gamma^5 = \begin{pmatrix} 0 & \sigma^z \\ \sigma^z & 0 \end{pmatrix}$$

"Effective Hamiltonian for 3D TI"

In addition we consider *antiferromagnetism (AFM)*

R. Li et al. ’10

Suppose electrons at Bi are AFM order



In addition we consider *antiferromagnetism (AFM)*

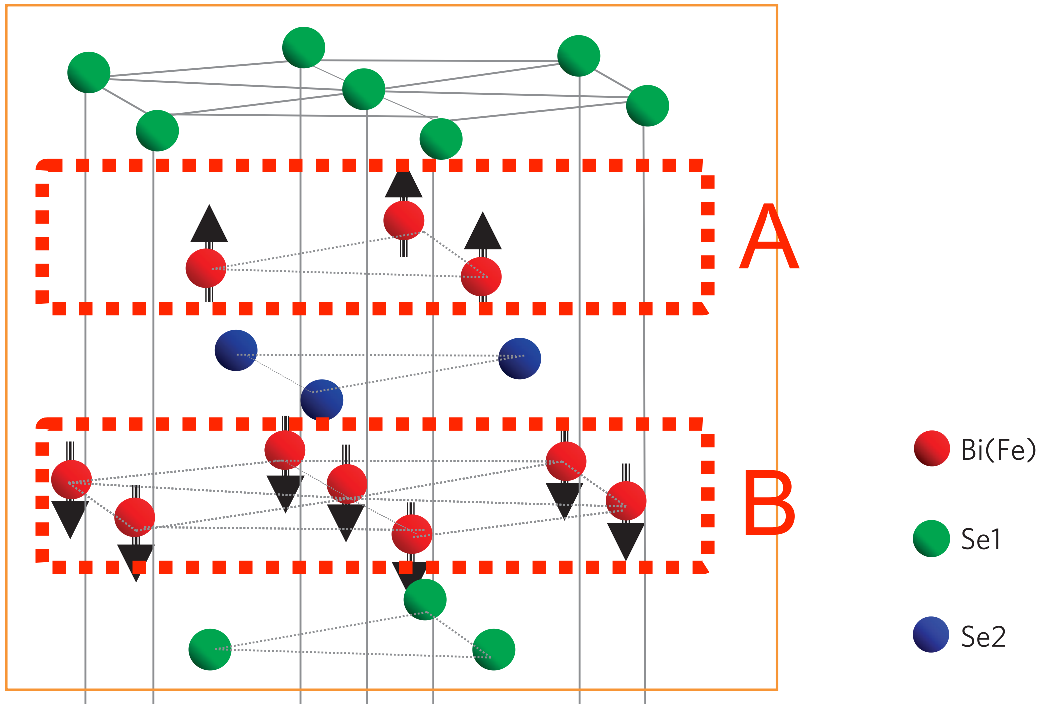
R. Li et al. '10

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

"Hubbard term"

U : parameter to give AFM

Large U ⟶ AFM



V : volume

N : number of site

$$n_{\rm A\sigma} = \psi^\dagger_{\rm A\sigma} \psi_{\rm A\sigma}$$

$$n_{\rm B\sigma} = \psi^\dagger_{\rm B\sigma} \psi_{\rm B\sigma}$$

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

↓

Hubbard-Stratonovich (HS) transformation

~ Inverse of integrating out a scalar

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

↓ Hubbard-Stratonovich (HS) transformation

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

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

↓ Hubbard-Stratonovich (HS) transformation

- A dynamical scalar ϕ that gives $\Gamma^5 d_5$ ($d_5 = \phi$)
- Mass term of ϕ ← missed in Sekine, Nomura '16, Sekine, Nomura '20, Schütte-Engel '21

(confirmed by private communication with Sekine-san)

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

↓ Hubbard-Stratonovich (HS) transformation

- A dynamical scalar ϕ that gives $\Gamma^5 d_5$ ($d_5 = \phi$)
- Mass term of ϕ
- ϕ relates to the axion field

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

R. Li et al. '10

Partition function (TI + AFM)

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

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

$$H = H_0 + \delta H$$

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

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

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$\Gamma^5 \phi$

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Summing over ψ , $\psi^\dagger$

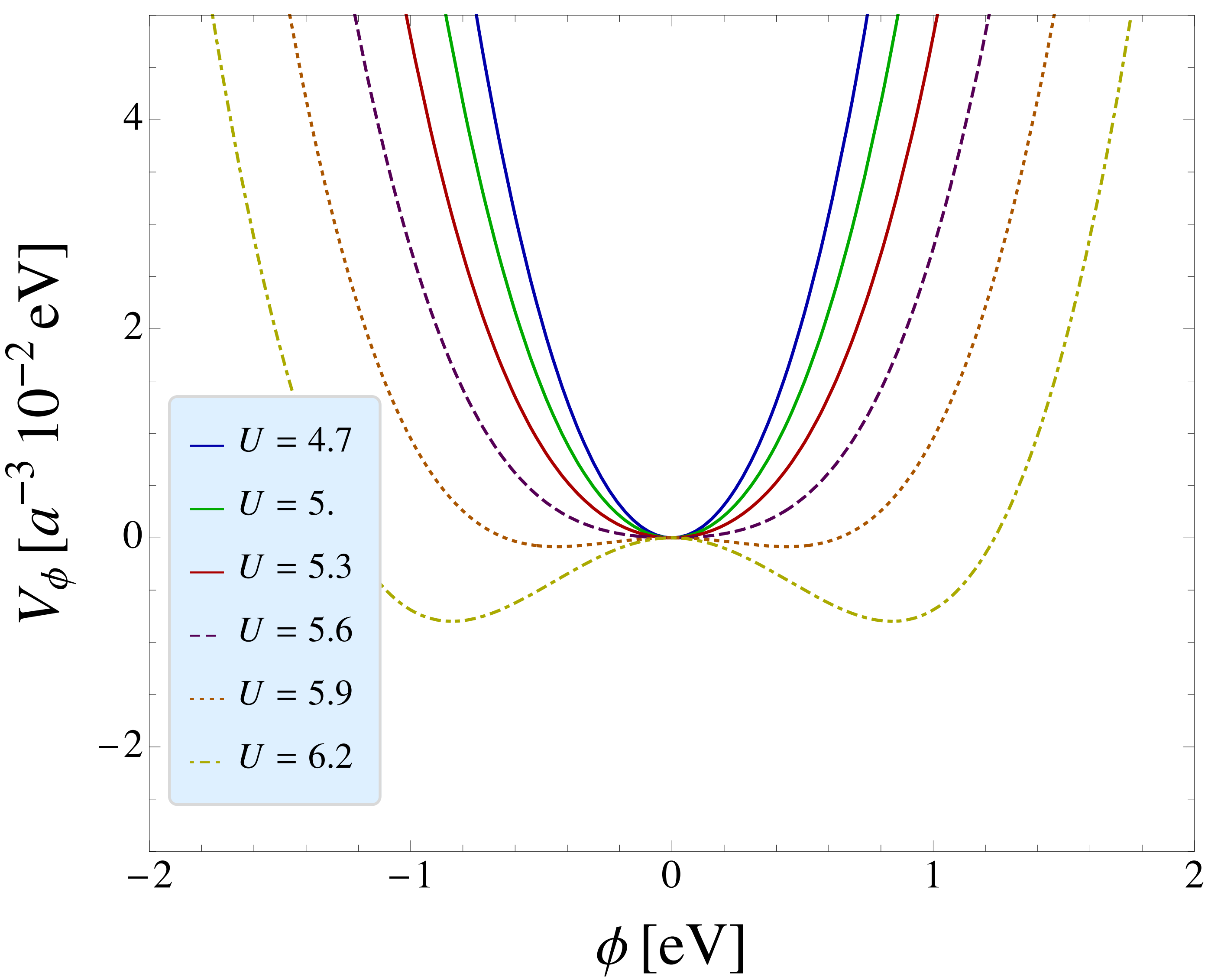
Effective potential for ϕ

Effective potential for θ

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

KI '21

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



$A_1 = A_2 = 1$

$B_1 = B_2 = -0.5$

KI ’21

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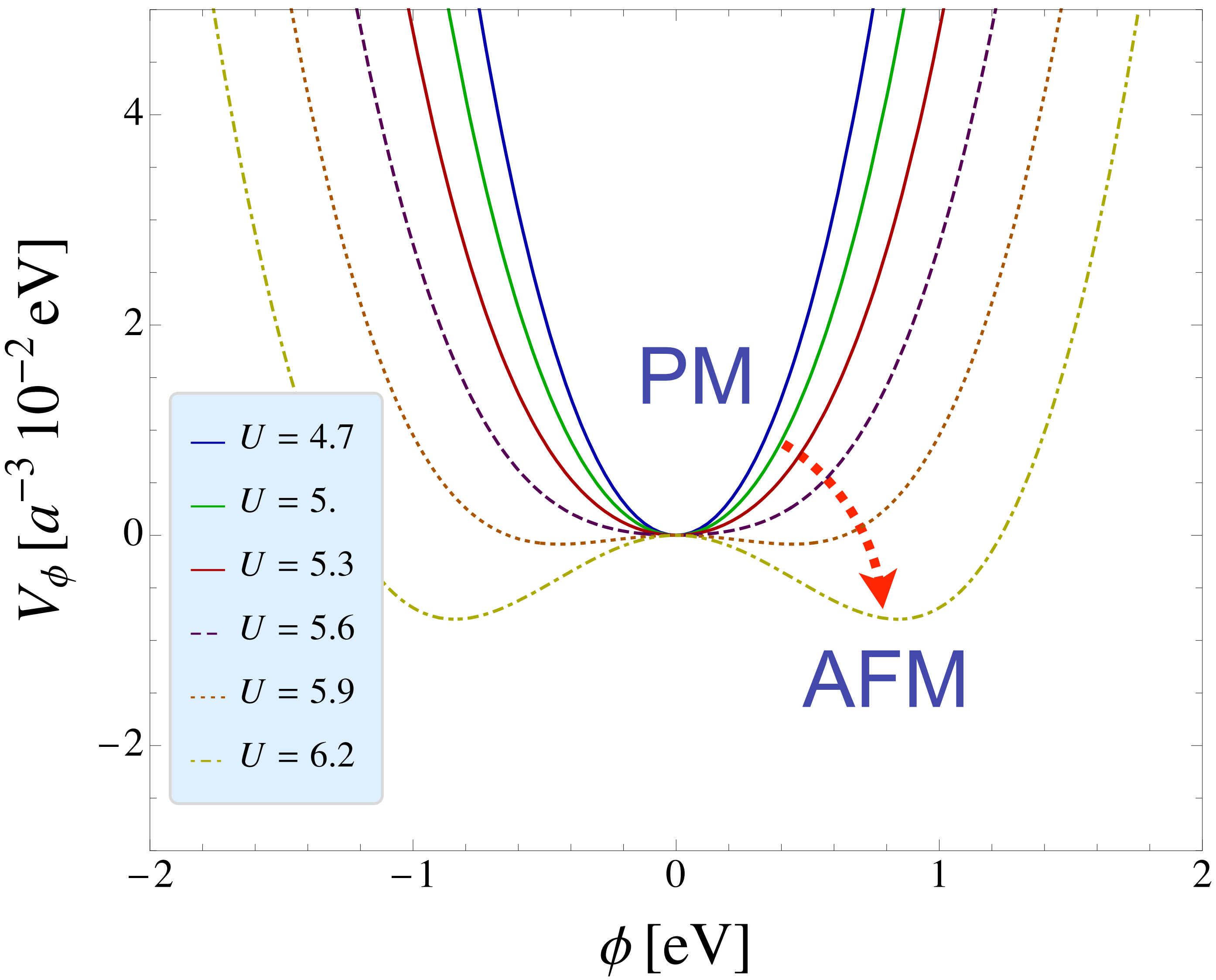

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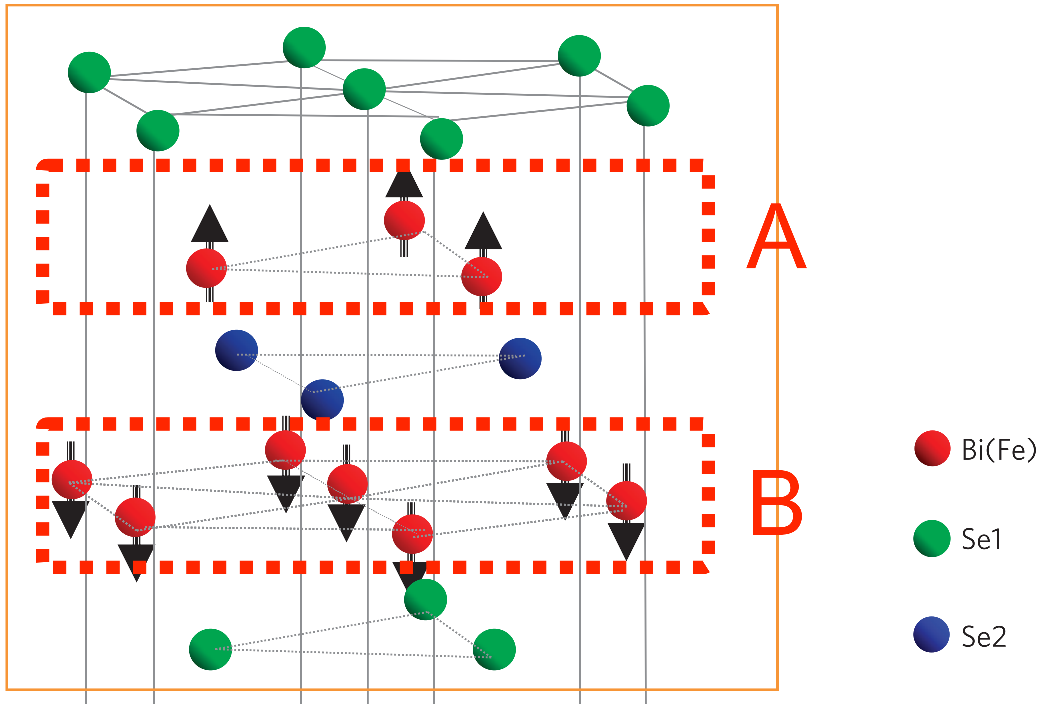


$$\langle \phi \rangle \sim \langle S_A \rangle = -\langle S_B \rangle$$

VEV of ϕ is the order parameter of AFM

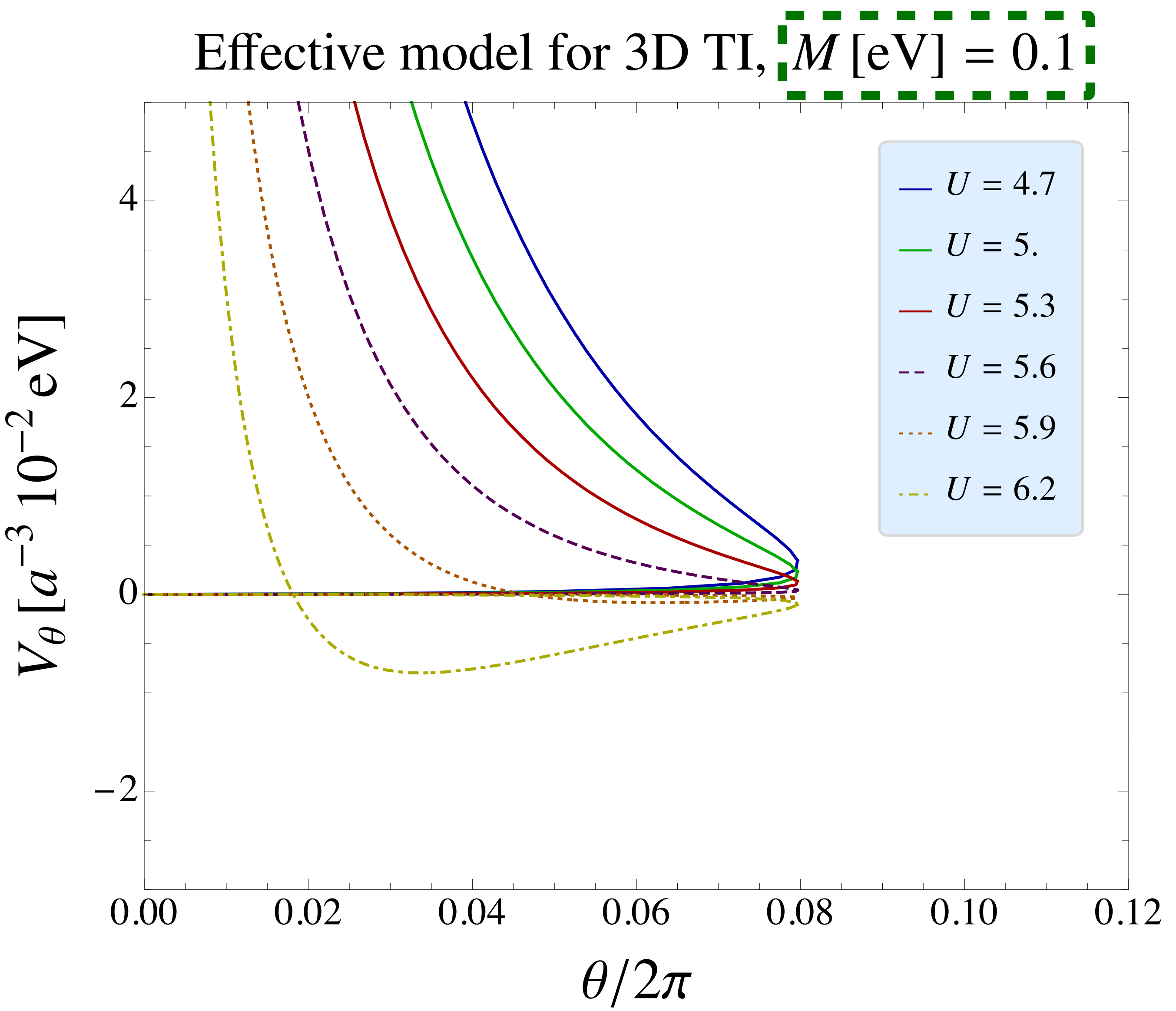
- $\langle \phi \rangle = 0$ → PM order
- $\langle \phi \rangle \neq 0$ → AFM order

PM (paramagnetic)

Effective potential in terms of θ

KI '21

NI phase



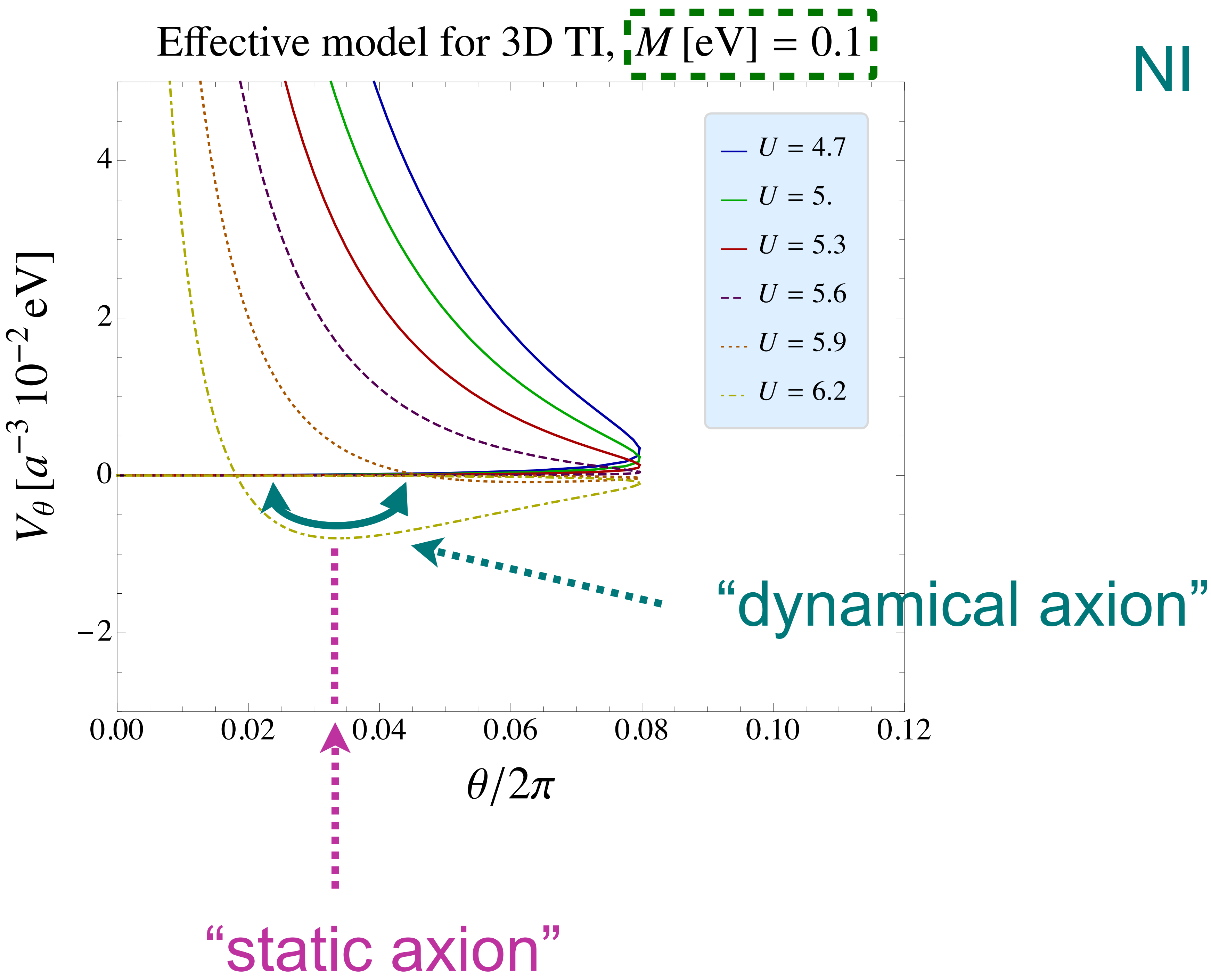
Potential minimum:

- $\theta = 0$ (PM)
- $\theta \neq 0$ (AFM)

Effective potential in terms of θ

KI '21

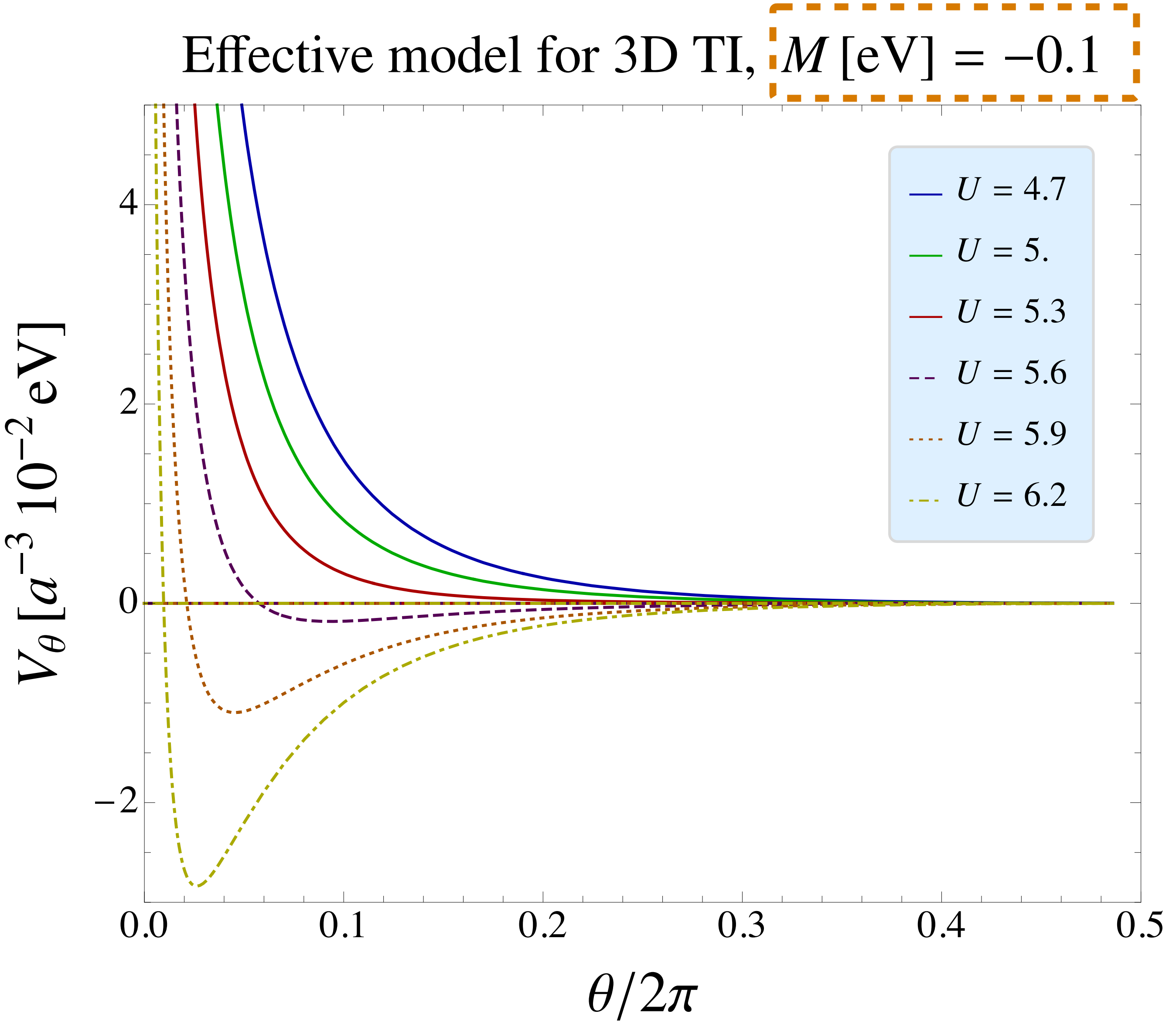
NI phase



Effective potential in terms of θ

KI '21

TI phase



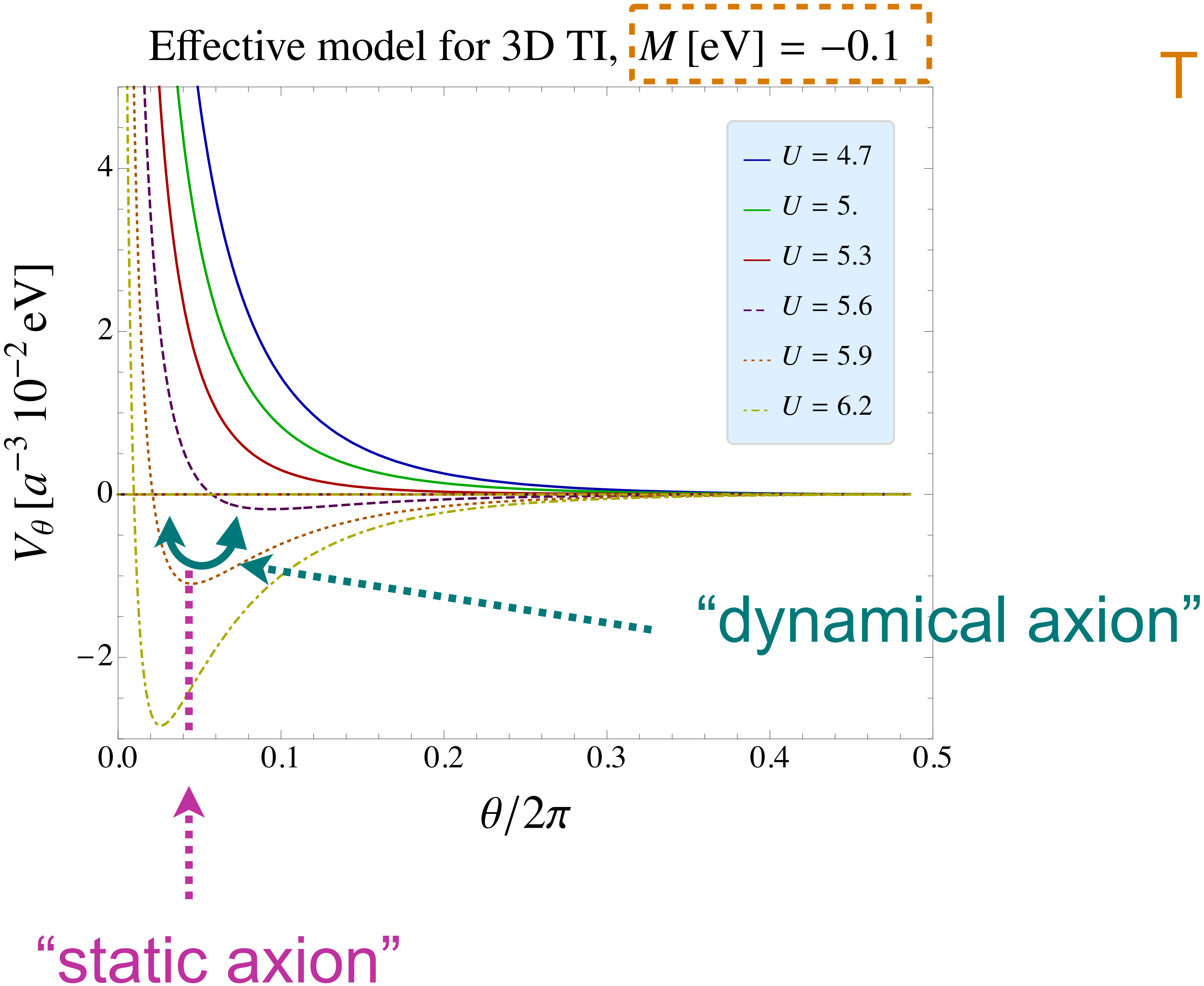
Potential minimum:

- $\theta = \pi$ (PM)
- $\theta \neq 0$ (AFM)

Effective potential in terms of θ

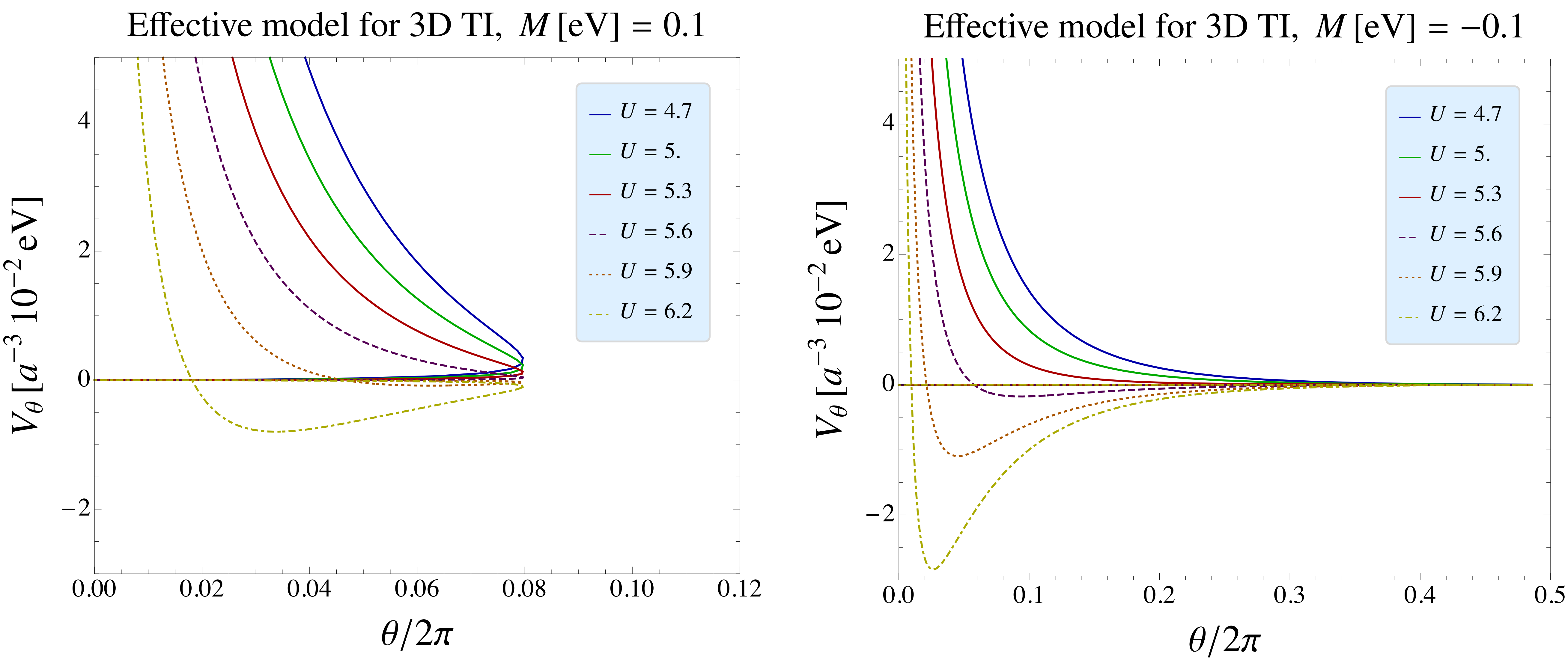
KI '21

TI phase



Axion in antiferromagnetic insulators

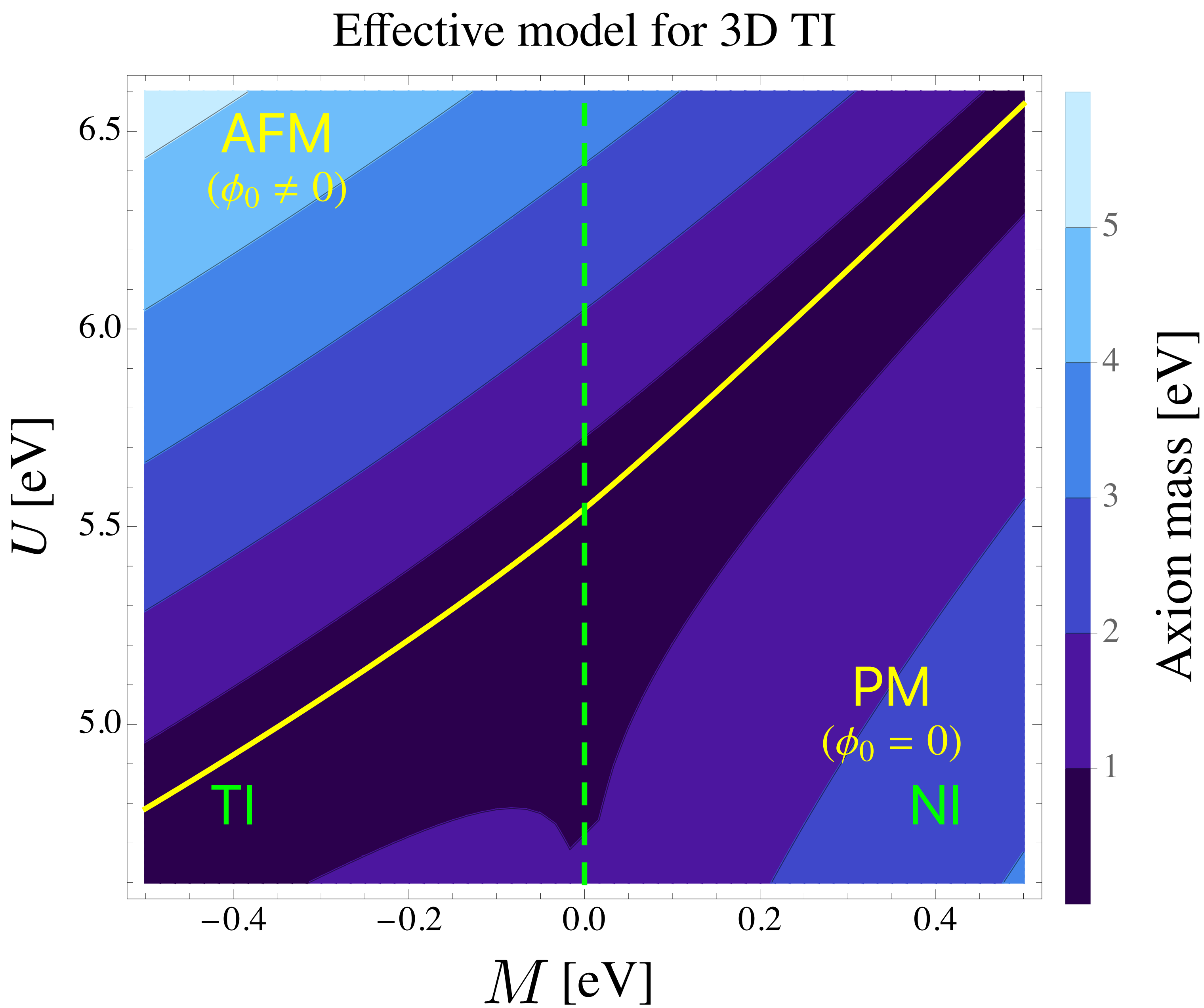
KI ’21



Dynamical axion exits in both TI and NI phases

Axion mass

KI '21



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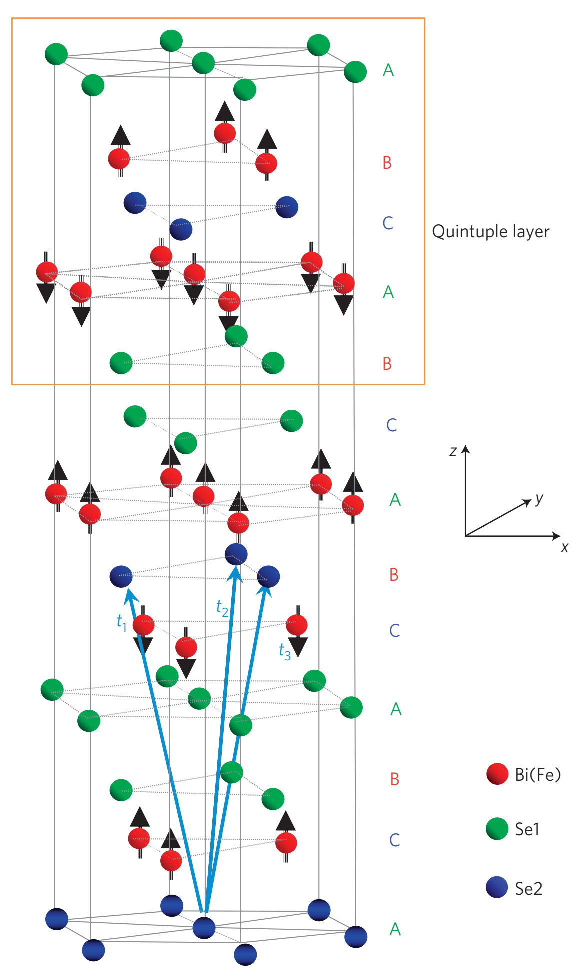

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Axion mass ~ $\mathcal{O}(\mathrm{meV})$

?

The thing would be …

R. Li et al. ’10

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

  (i.e., $\langle \phi \rangle$ is considered to be a free parameter)

- AFM order is *assumed*

The thing would be …

R. Li et al. '10

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

  (i.e., $\langle\phi\rangle$ is considered to be a free parameter)

  ⟶ Axion mass ~ $\mathcal{O}(\mathrm{meV})$ $(\because \ m_a^2 \propto m_5^2)$

But this is naively difficult since

- AFM order is *assumed*

$m_5 \sim U \sim \mathrm{eV}$ (in AFM order)

The thing would be …

R. Li et al. ’10

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  No AFM in TI in the first place

  ⟶ Fe-doped $\mathrm{Bi_2Se_3}$ is considered

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  ⟶ Fe-doped $\mathrm{Bi_2Se_3}$ is considered

  "likely to be AFM" J.M. Zhang et al. '13

  (by first-principles calculation)

  ⟶ It looks unlikely to be realized

The thing would be …

R. Li et al. '10

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

  (i.e., $\langle \phi \rangle$ is considered to be a free parameter)

  ⟶ Axion mass ~ $\mathcal{O}(\mathrm{meV})$ $\quad (\because \ m_a^2 \propto m_5^2)$

⟶ Consistent determination of $\langle \phi \rangle$ is crucial for axion mass

- AFM order is *assumed*

  No AFM in TI in the first place

  ⟶ Fe-doped $\mathrm{Bi_2Se_3}$ is considered

J.M. Zhang et al. '13

4. Conclusions

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

- Dynamical axion appears both in TI and NI
- Axion mass is $\lesssim \mathcal{O}(\mathrm{eV})$
- Material search is crucial for the future axion search

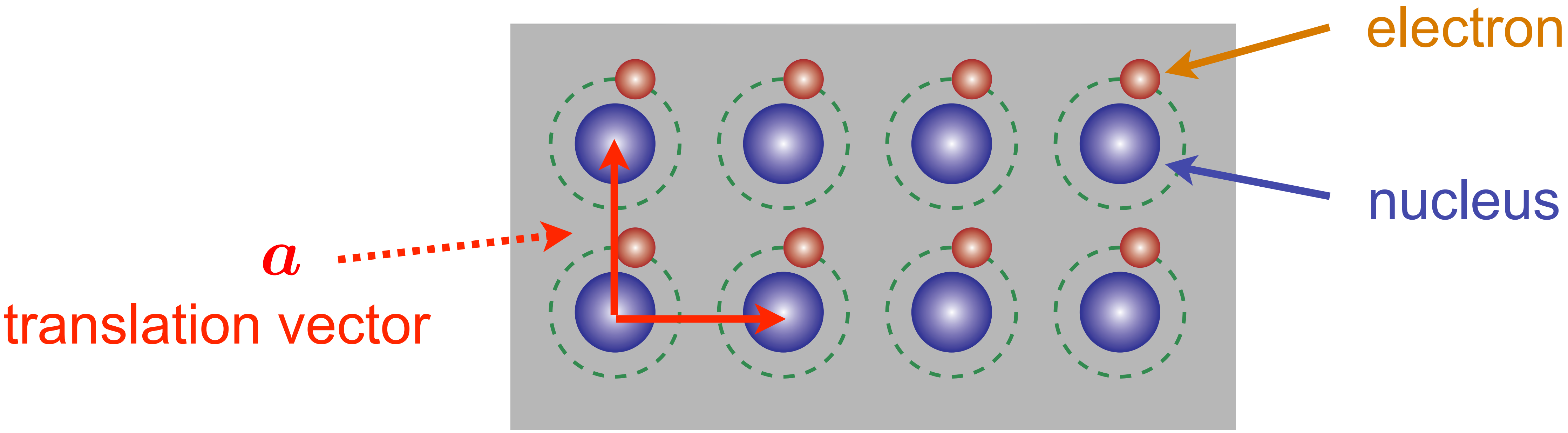
Discussion

- How do we describe axion in $\mathrm{Mn_2Bi_2Te_5}$?
- What about axion in NI ?
- Dynamical axion in ferromagnetic state or other magnetic states?

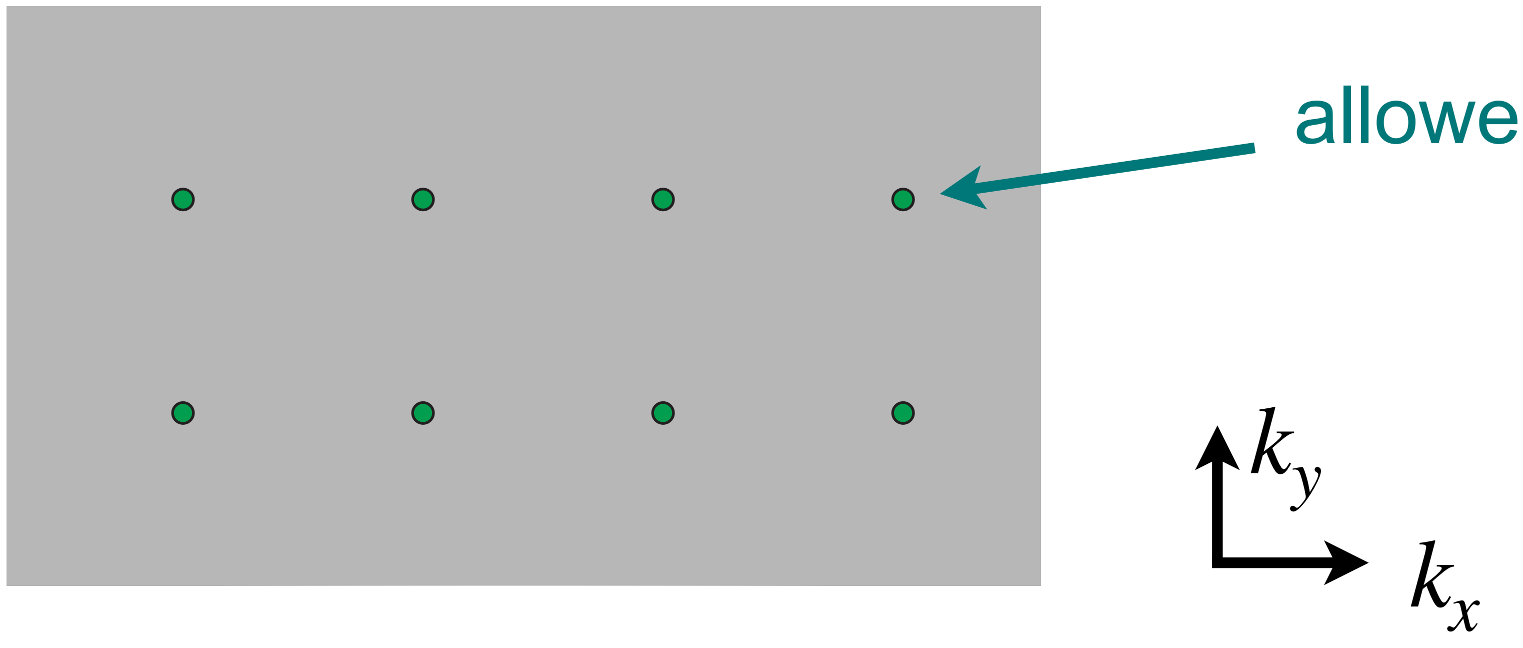
Backups

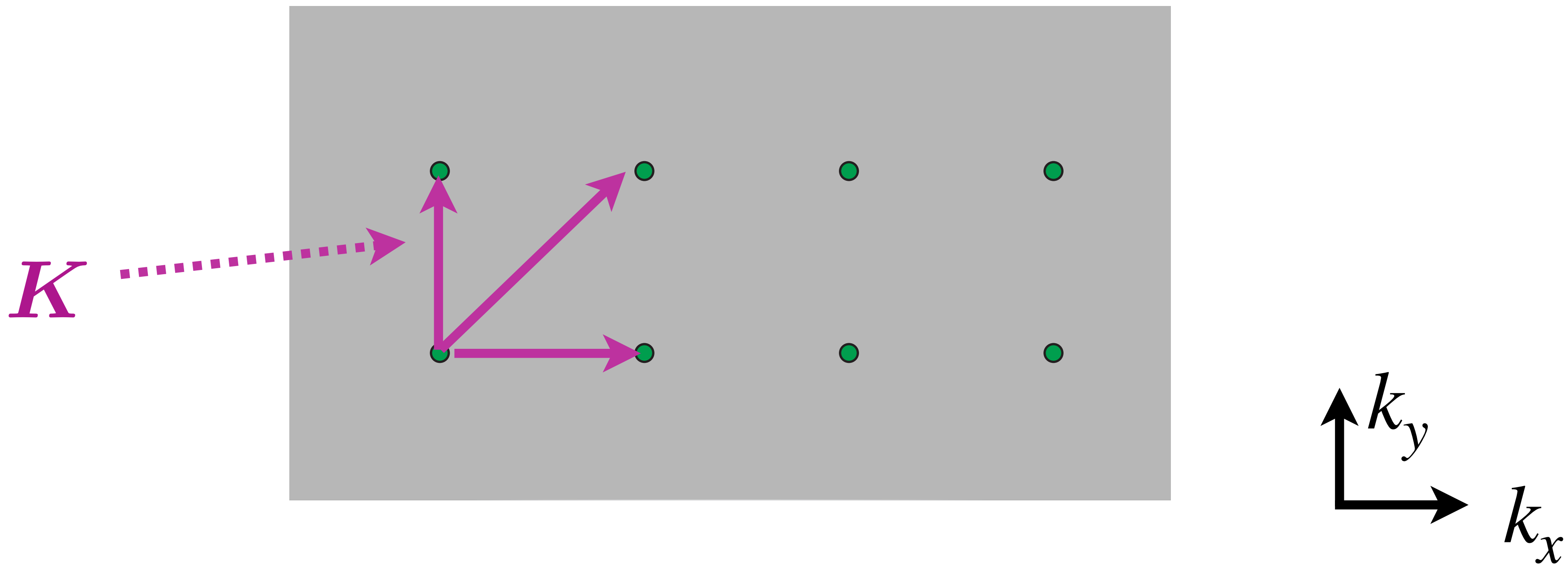
Basics

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



- Consequently there is periodicity in the wavenumber space





- Periodicity $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{a}$ corresponds to $\boldsymbol{k} \to \boldsymbol{k} + \boldsymbol{K}$

  ($\boldsymbol{K}$: 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

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

  (Bloch's theorem)

  Bloch function (state)

Thouless, Kohmoto, Nightingale, den Nijs '82

Hall conductivity:

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

TKNN formula

$$\nu \equiv \sum_n \int_{\mathrm{BZ}} \frac{d^2k}{2\pi} [\boldsymbol{\nabla}_{\boldsymbol{k}} \times \boldsymbol{a}_n(\boldsymbol{k})]_z$$

$$\boldsymbol{a}_n(\boldsymbol{k}) \equiv -i \langle u_{n\boldsymbol{k}} | \frac{\partial}{\partial \boldsymbol{k}} | u_{n\boldsymbol{k}} \rangle$$

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

n : label of band

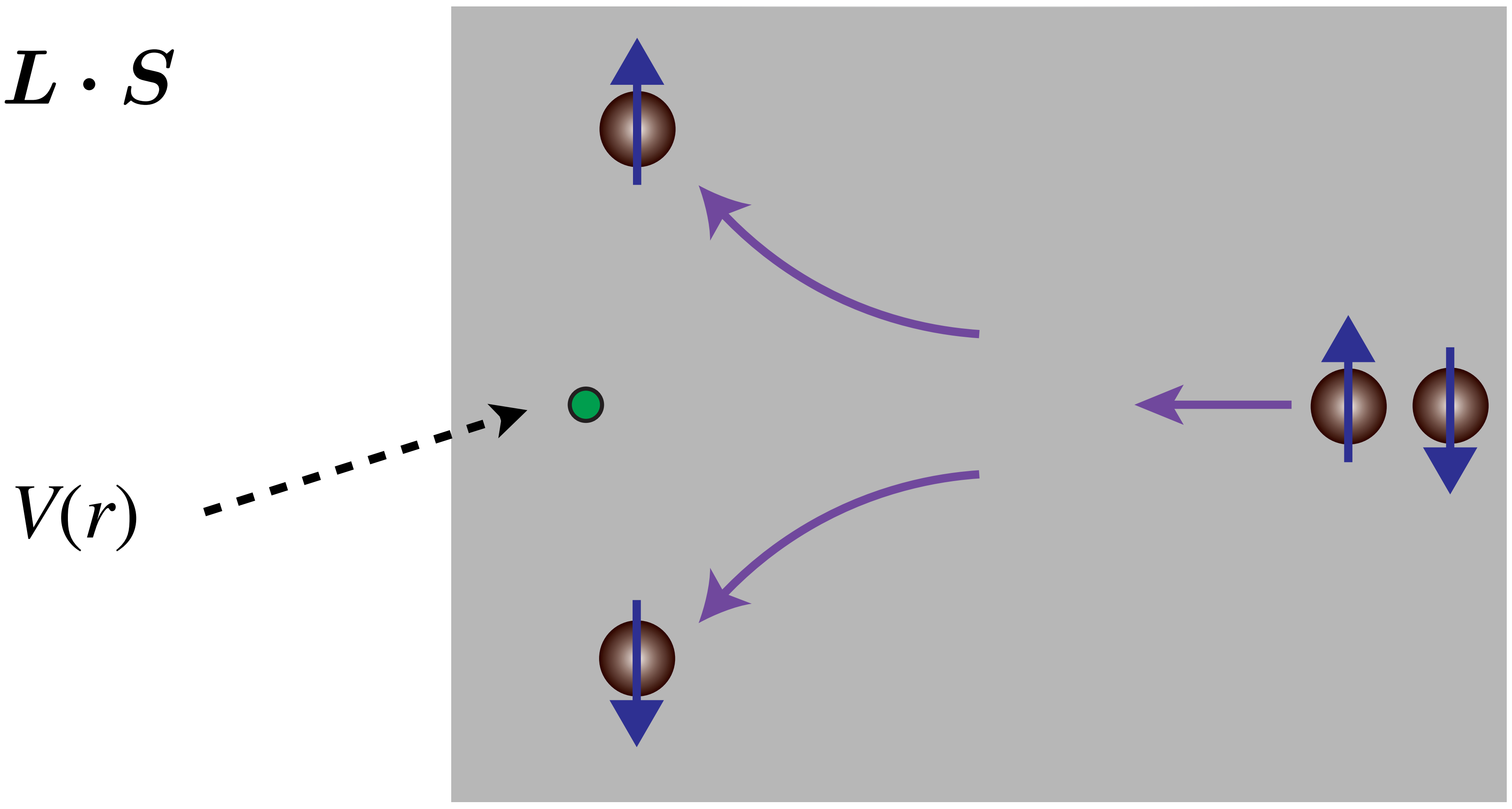
→ ν is given by (half-) integer

"(Integer) QH effect"

Spin-orbit coupling (SOC)

e.g.,

$$H_{\mathrm{SO}} = V(r)\boldsymbol{L}\cdot\boldsymbol{S}$$



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

Keywords for topological insulators

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

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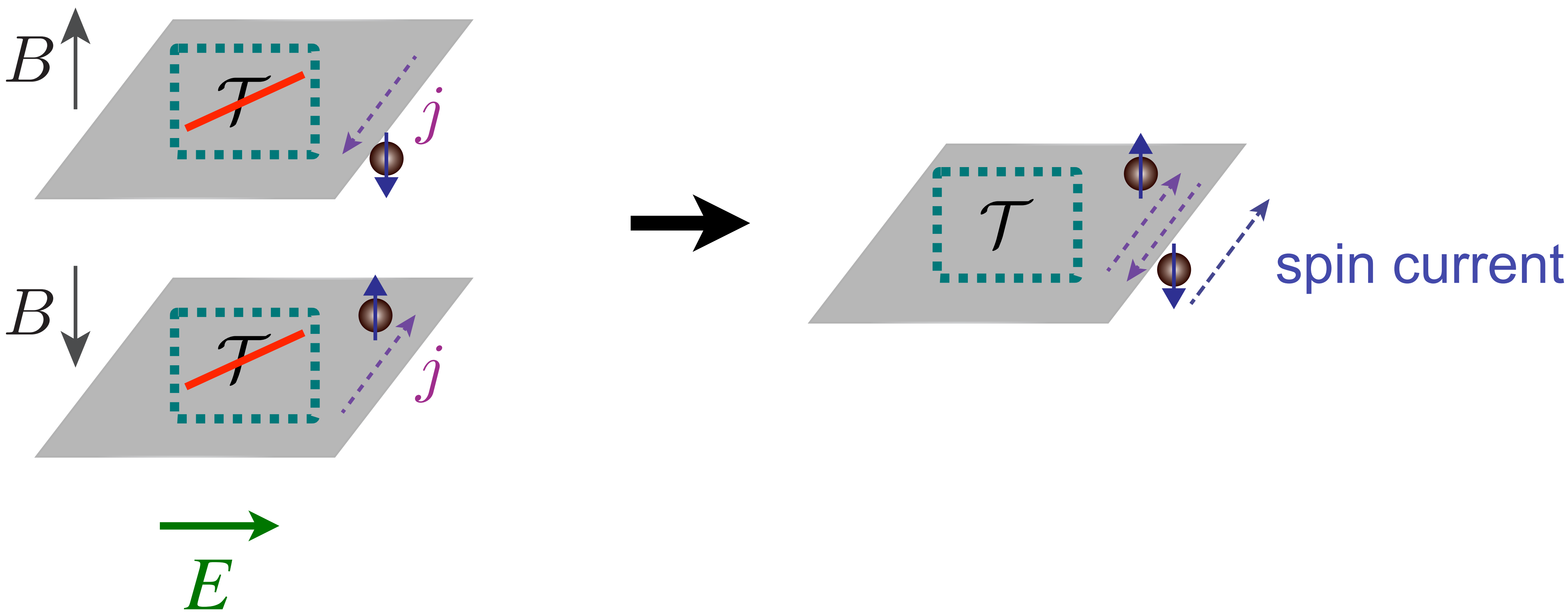
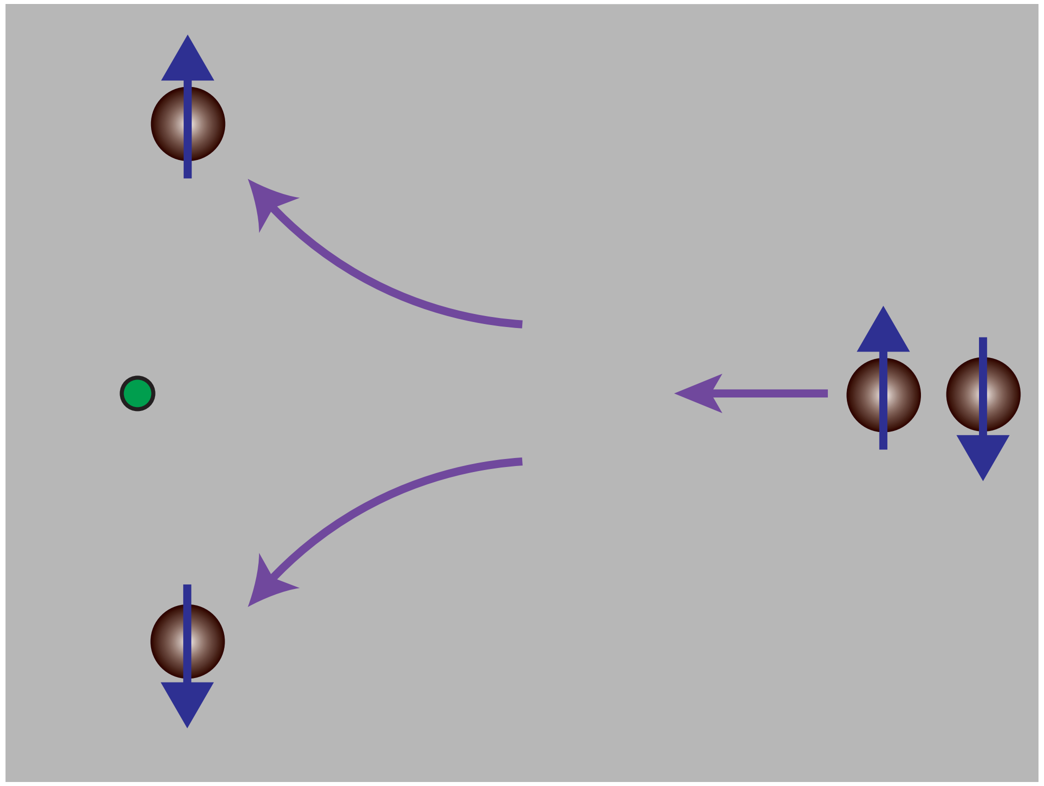


B breaks $\mathcal{T}$ but the combination of B and $-B$ keeps $\mathcal{T}$

Keywords for topological insulators

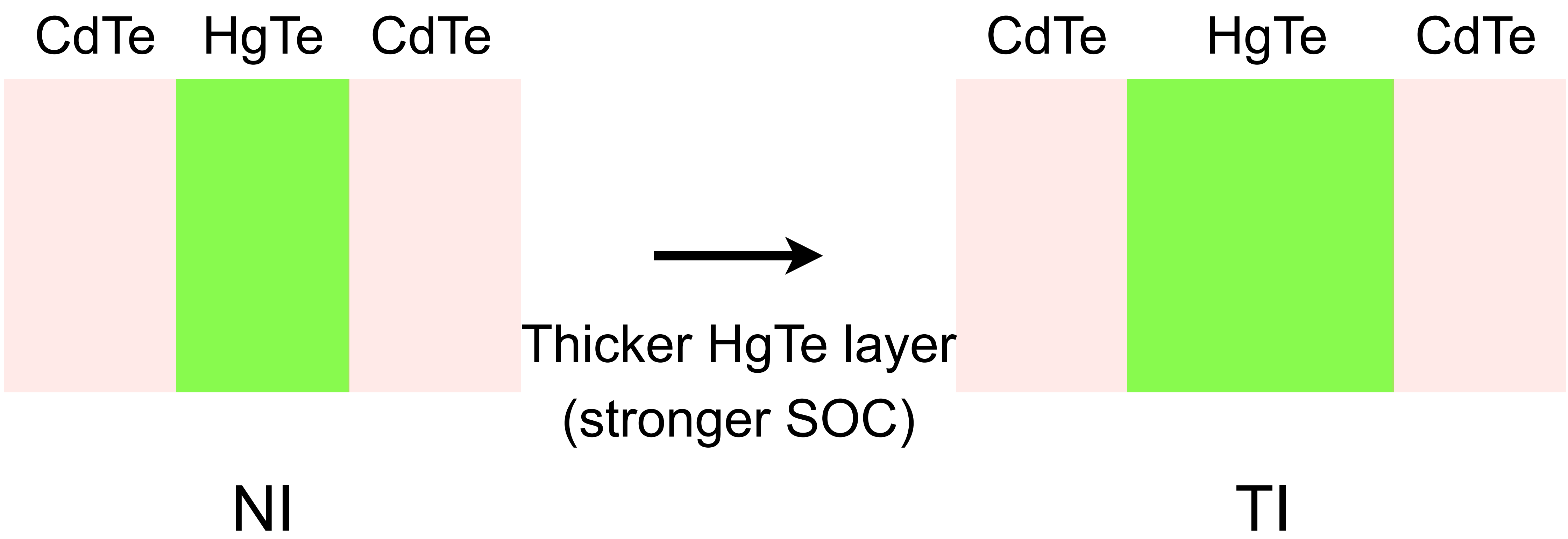
- Time reversal invariance ($\mathcal{T}$)
- Strong spin-orbit coupling (SOC)



Strong SOC is crucial for the realization

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

König et al. ’07



Band inversion happens in the energy band of HgTe

Magnetoelectric (ME) effect

predicted by Landau&Lifshitz

discovered by Dzyaloshinskii '60

- Electric field ($\boldsymbol{E}$) induces magnetization $\boldsymbol{M}$
- Magnetic field ($\boldsymbol{B}$) induces electric polarization $\boldsymbol{P}$

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

$\longleftarrow$

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

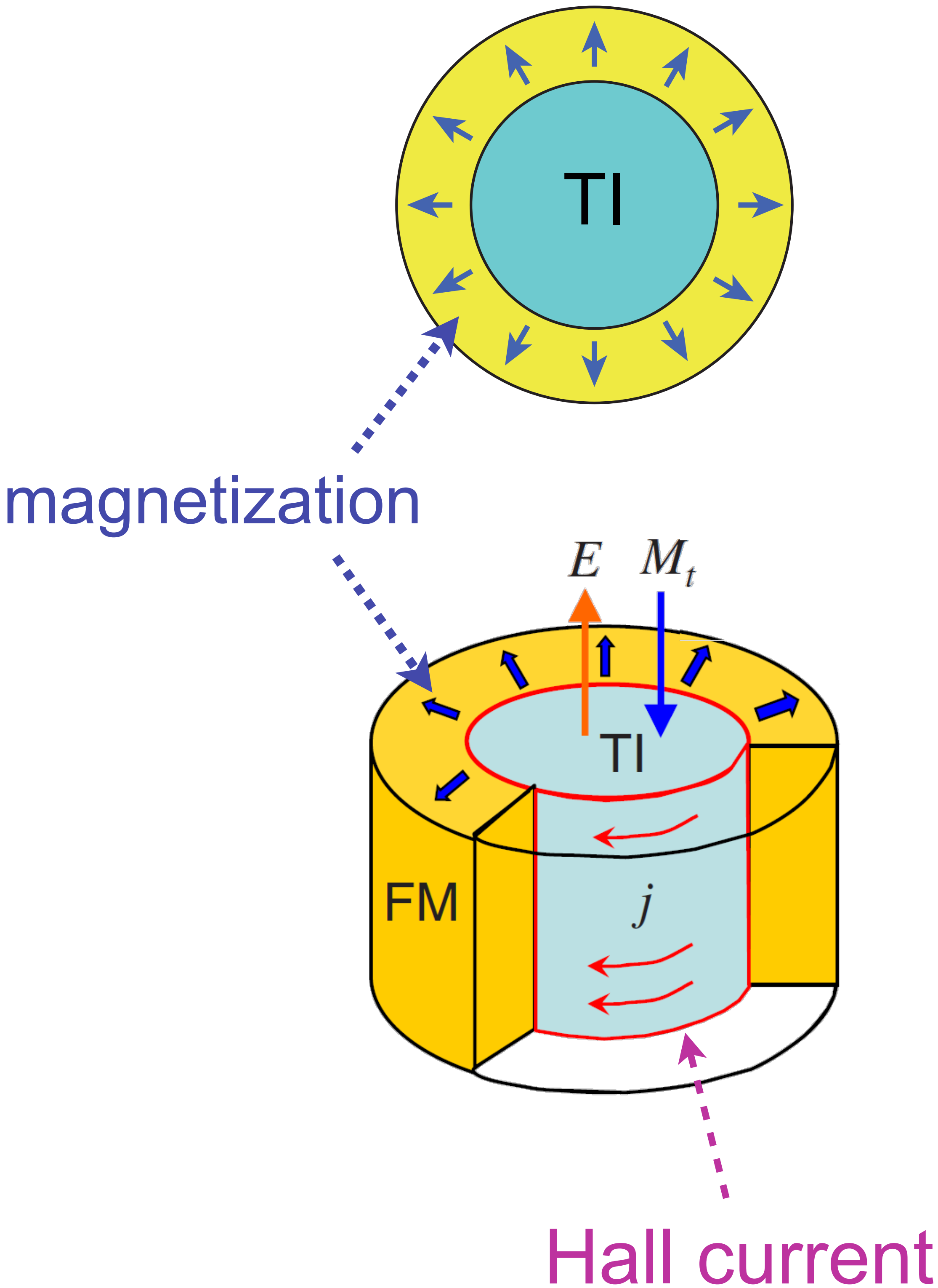
$$M_i = -\frac{1}{V} \left. \frac{\partial F}{\partial E_i} \right|_{B=0}$$

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

α_{ij} : constant

3D TI cylinder coated with magnetization directing outside

Qi, Hughes, Zhang '08



Half-integer AQH current

↓

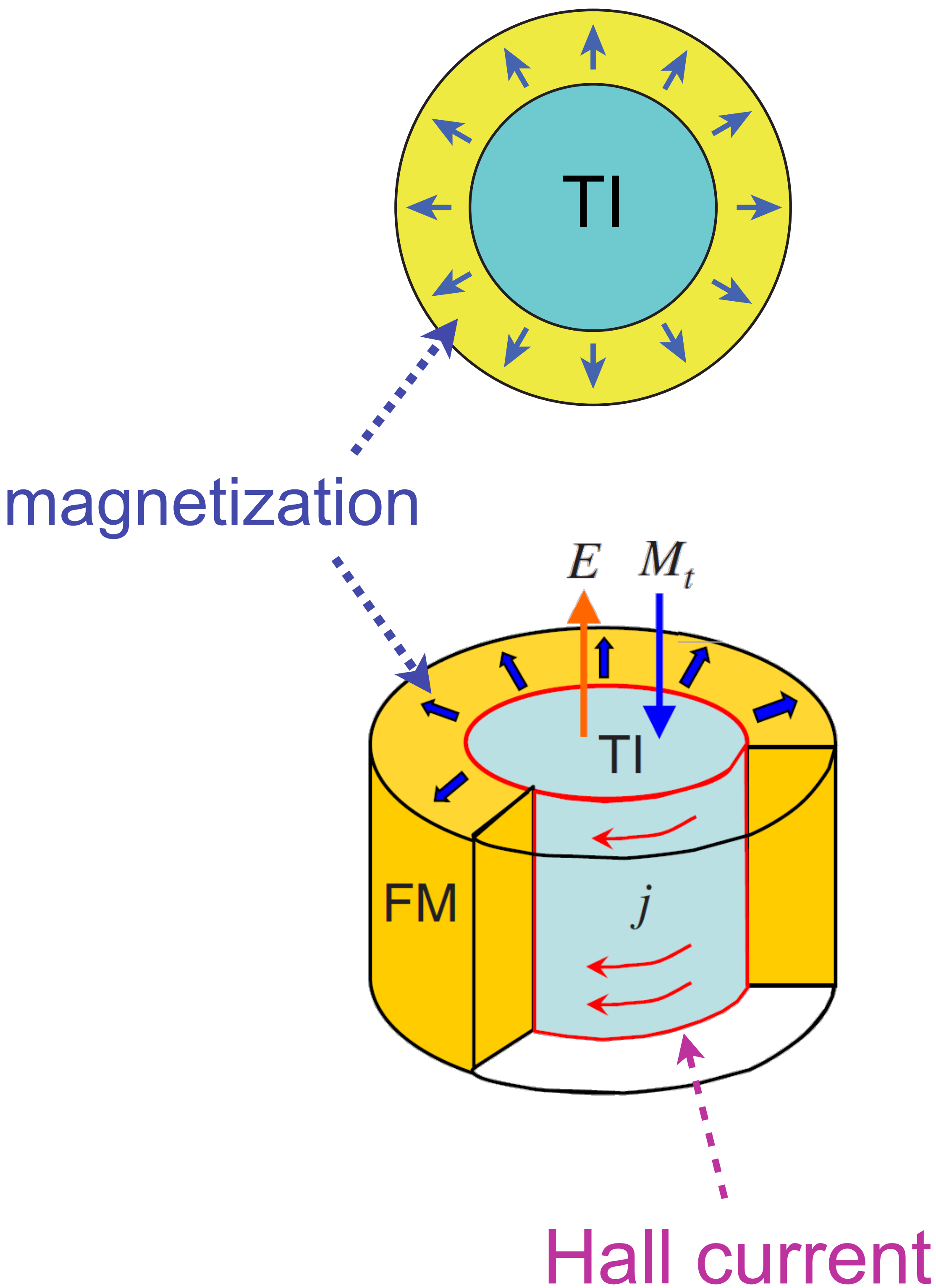
The current induces magnetization in z direction

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

α : fine-structure constant

3D TI cylinder coated with magnetization directing outside

Qi, Hughes, Zhang '08



Half-integer AQH current

↓

The current induces magnetization in z direction

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

The coefficient is given by fine-structure constant

α : fine-structure constant

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

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

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

$\theta = \pm\,\pi$ is called static axion

($\theta = 0$ in NI)

Effective potential for ϕ

KI '21

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

Negative potential

The mass term stabilizes the potential

$$|d_0|^2 = \sum_{a=1}^{4} |d^a|^2$$

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

Derivation as chiral anomaly

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

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

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

Derivation as chiral anomaly

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

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

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

"Dirac model"

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

Unitary transformation of the basis

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

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

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

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

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

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

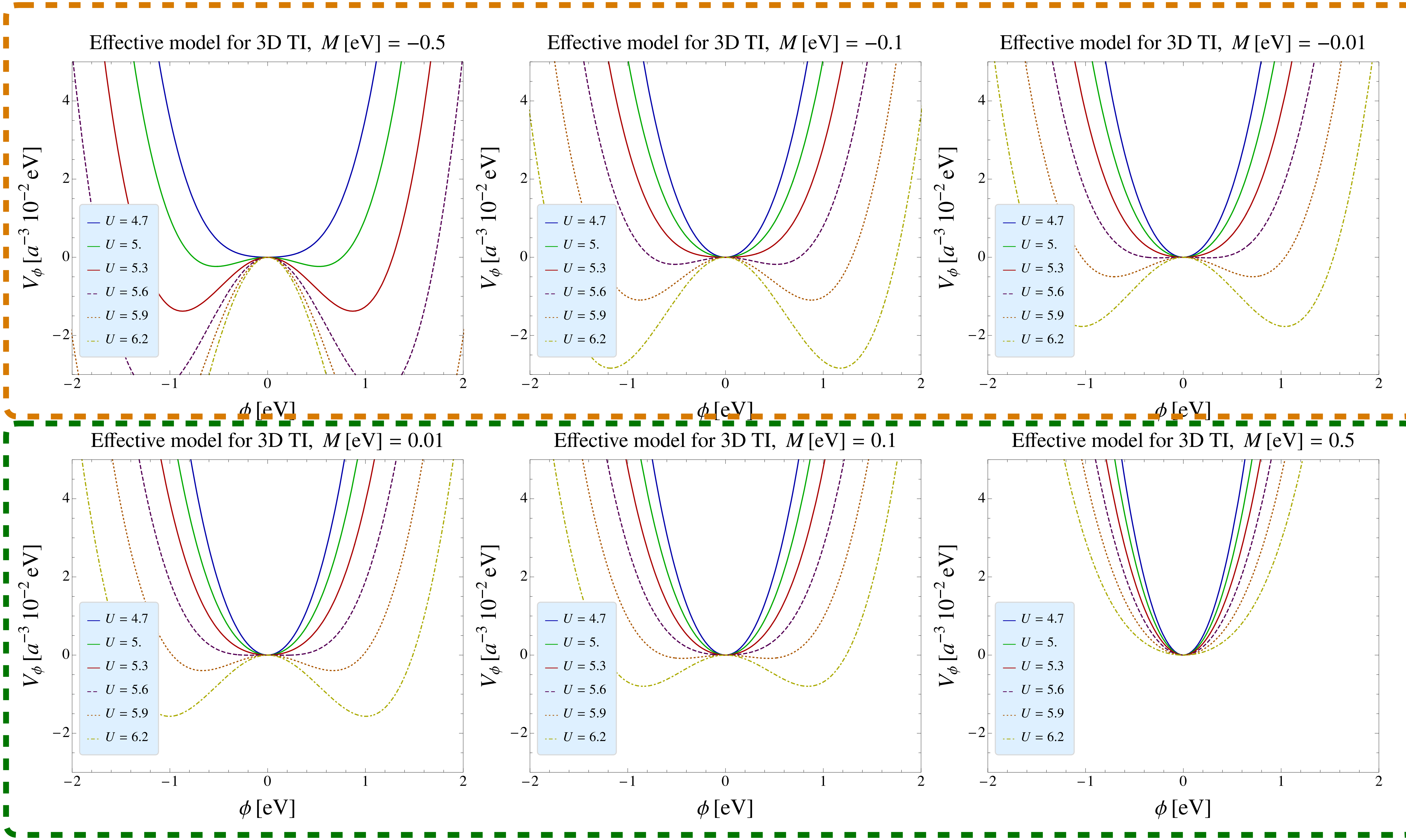
it is consistent with

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

M dependence

KI '21

TI

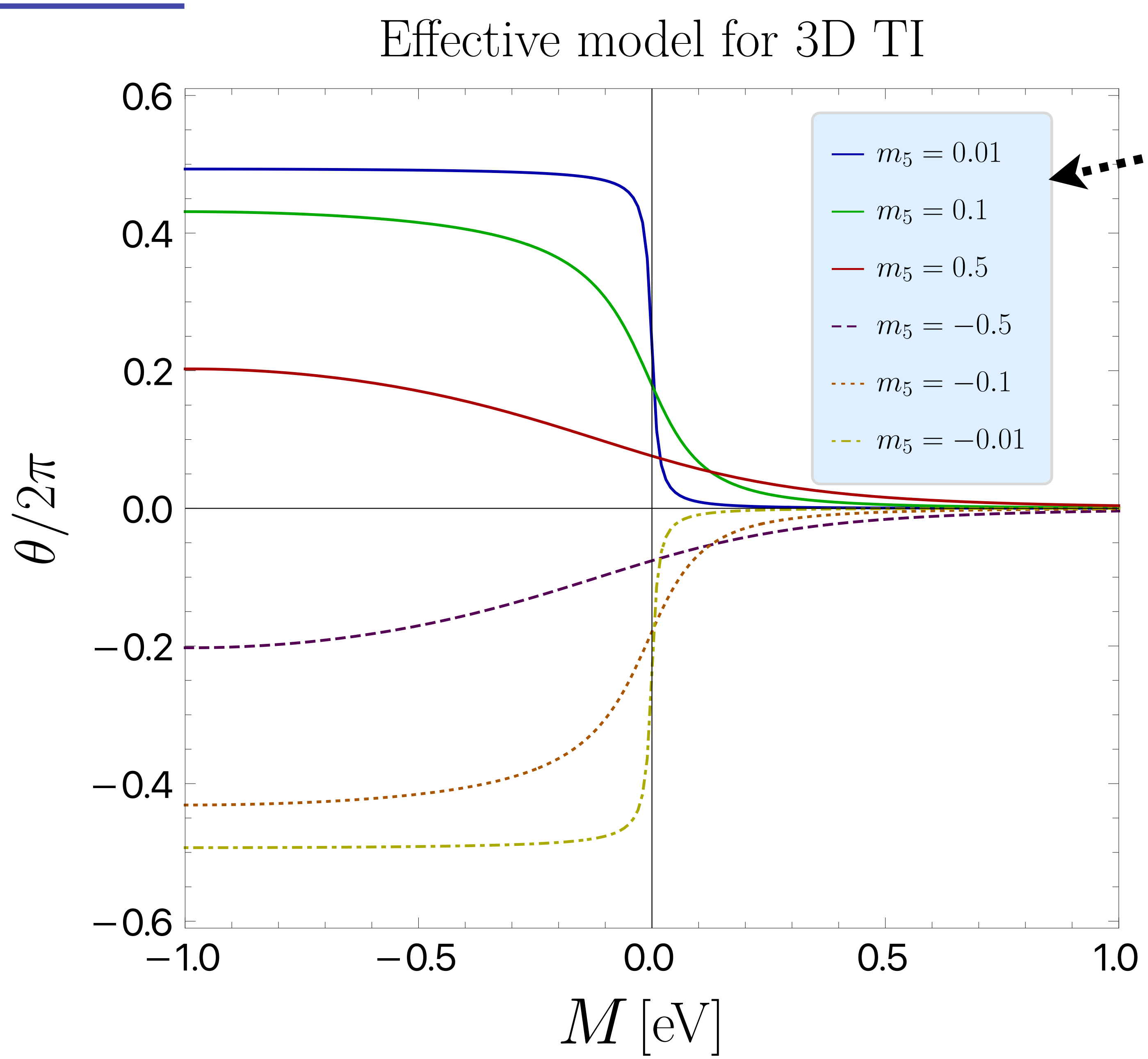


NI

The difference between TI and NI is not clear

θ as function of M

KI '21

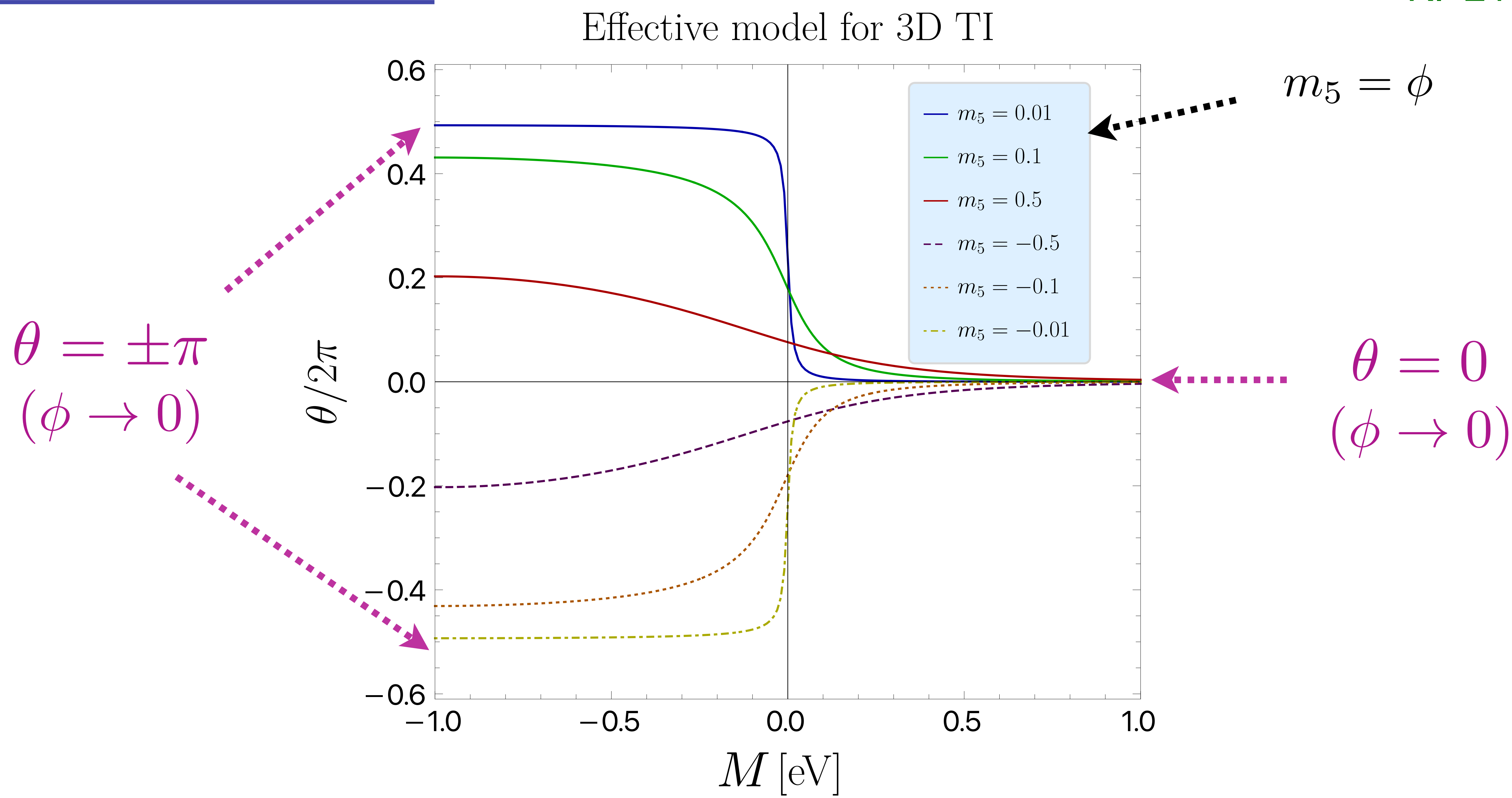


$m_5 = \phi$

calculation for Dirac model is done by Zhang '19

θ as function of M

KI '21

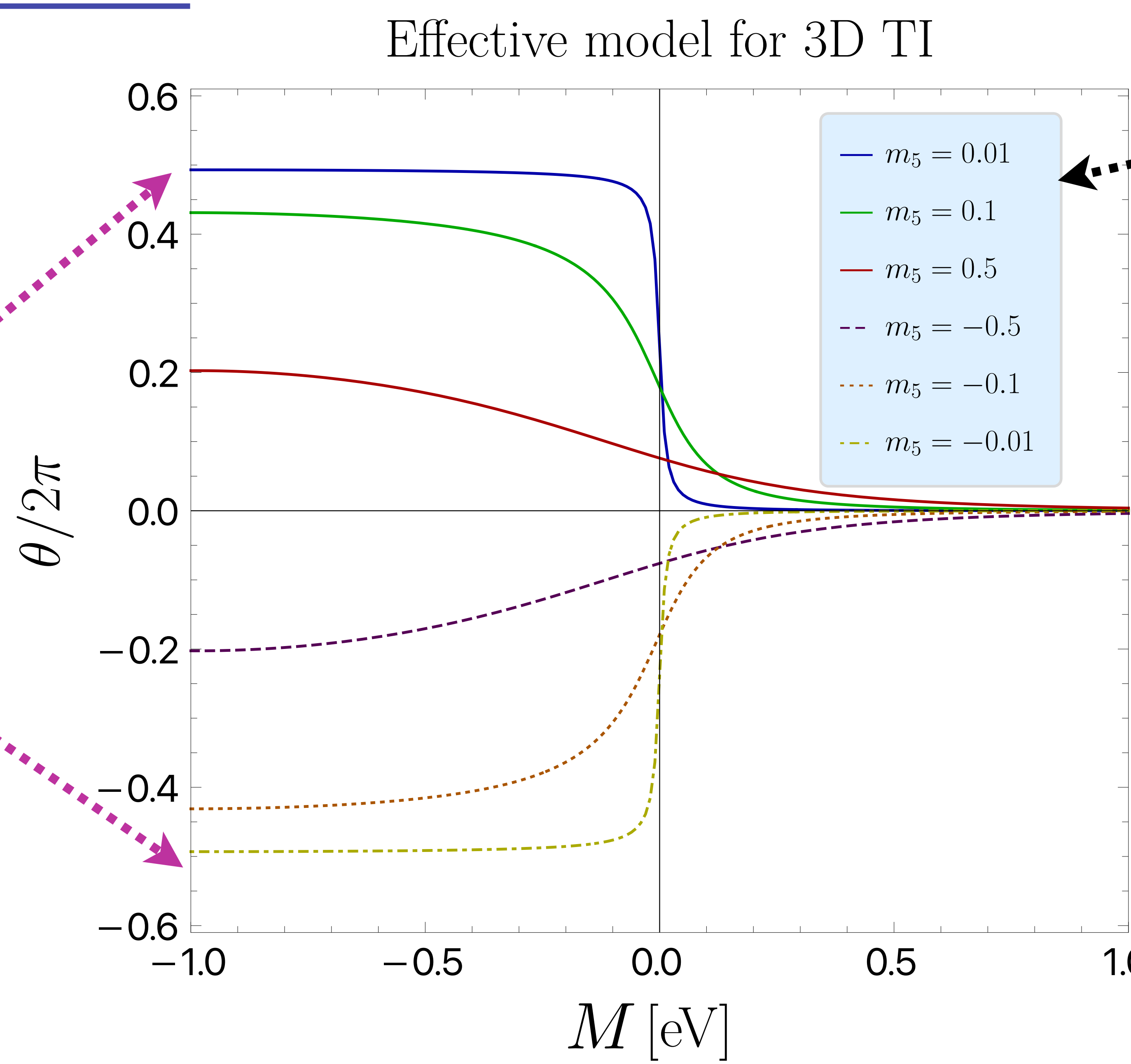


θ as function of M

KI '21

$m_5 = \phi$

$\theta = \pm\pi$
$(\phi \to 0)$



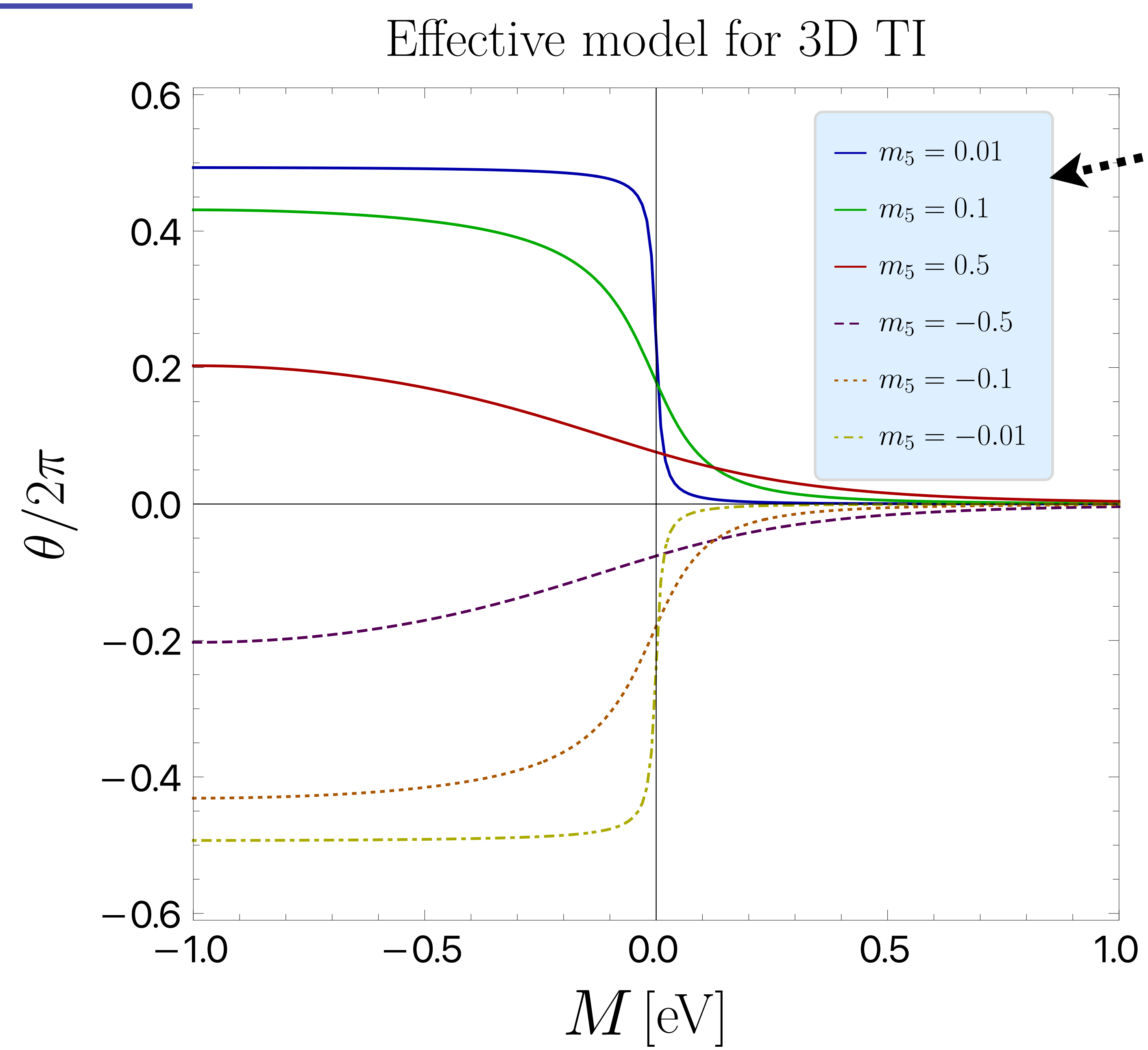
$\theta = 0$
$(\phi \to 0)$

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

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

θ as function of M

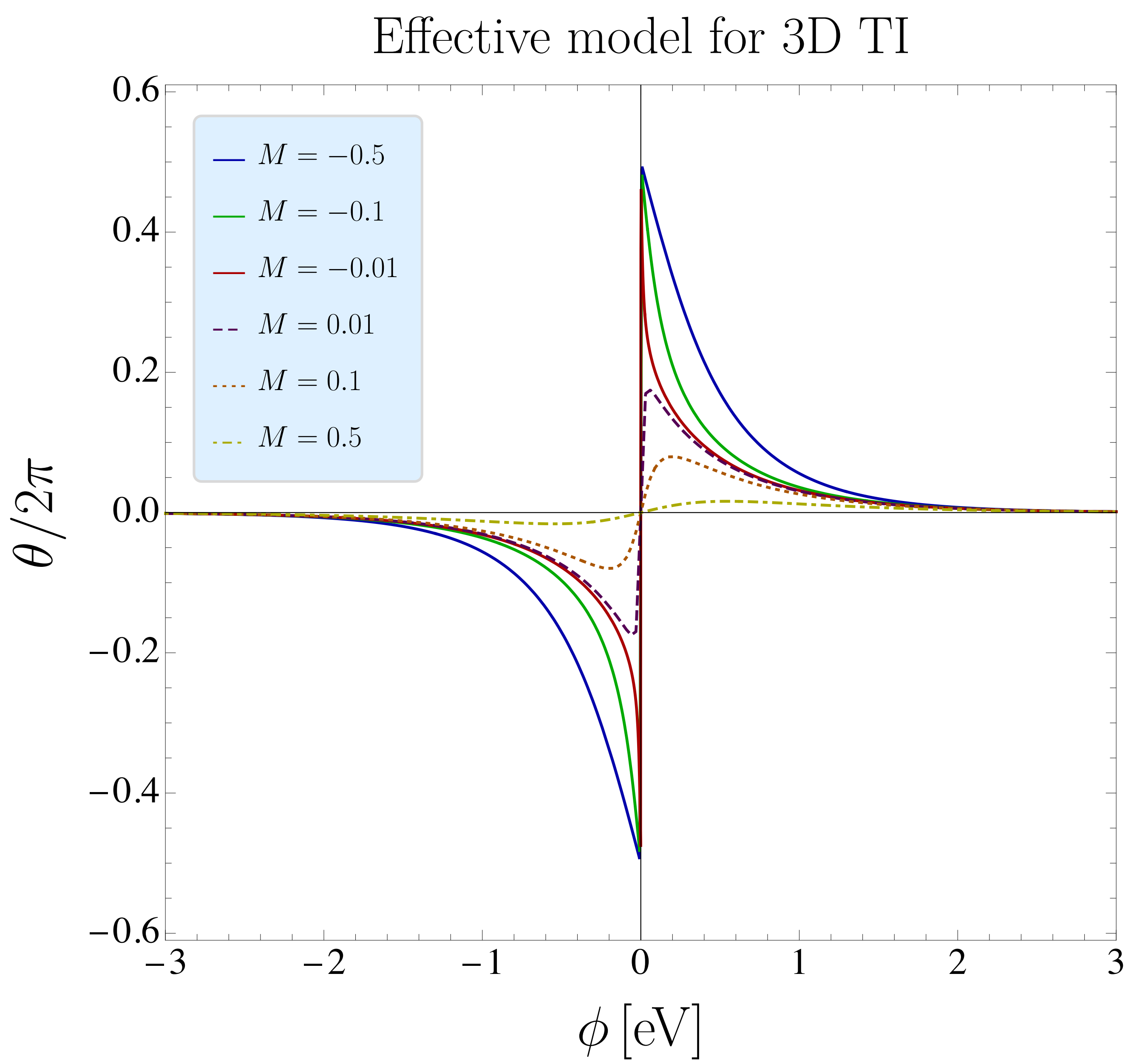
KI '21



$m_5 = \phi$

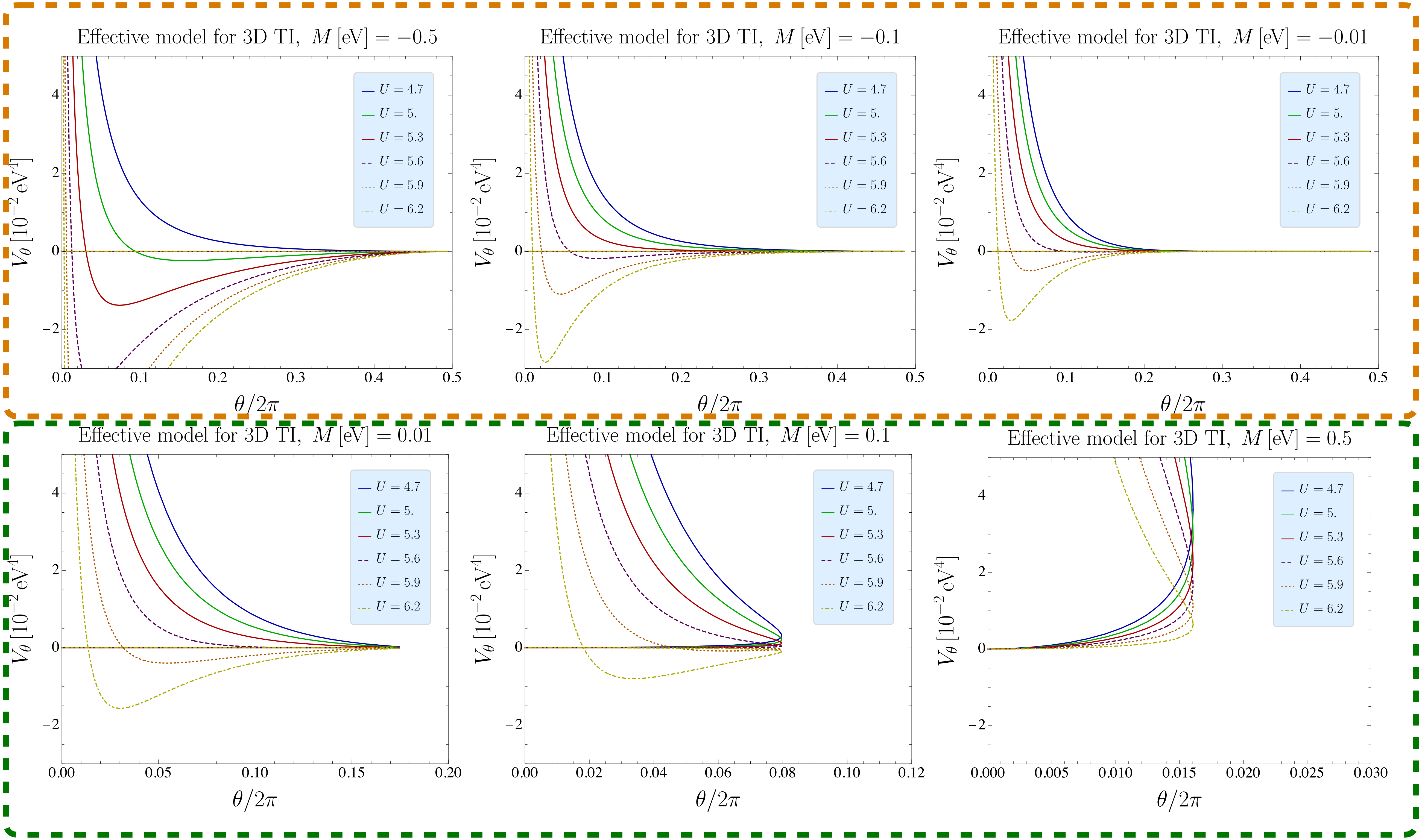
$\phi \neq 0$ ($\not{\mathcal{T}}$) ⟷ AFM order ⟶ θ takes continuum variable

θ as function of ϕ



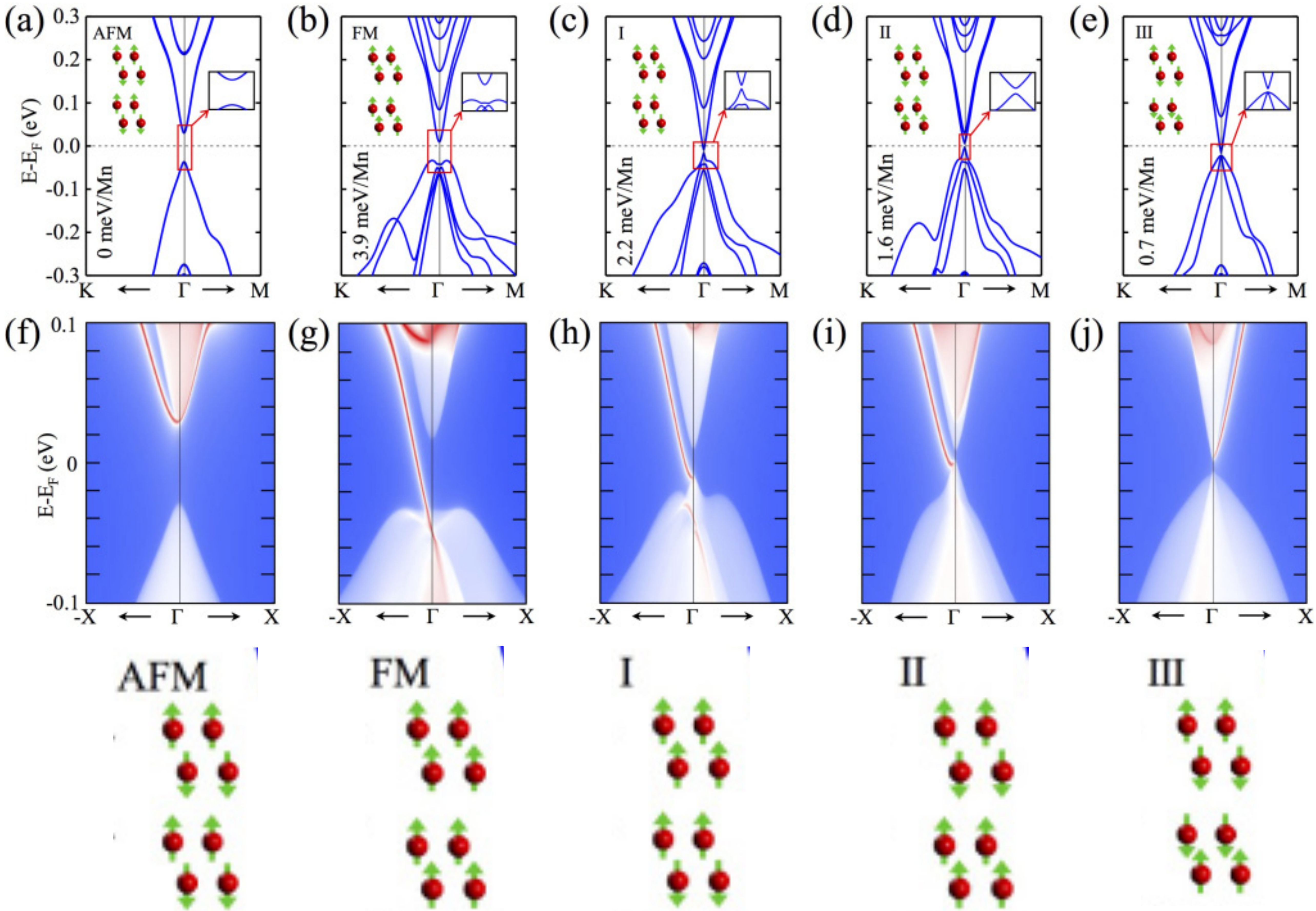
M dependence

TI



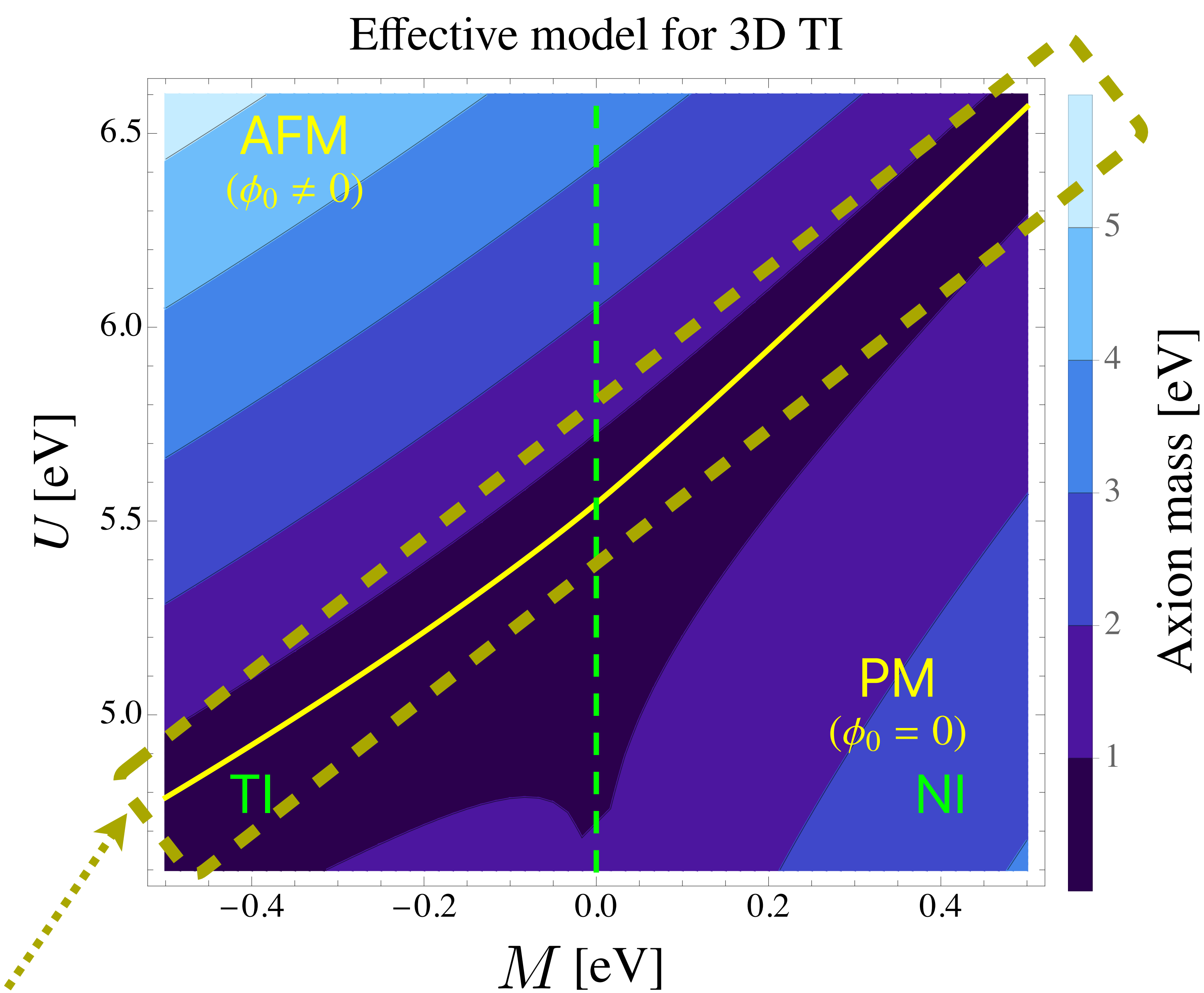
NI

Y. Li et al. '20



(a) (b) (c) (d) (e)
AFM
FM
I
II
III
0 meV/Mn
3.9 meV/Mn
2.2 meV/Mn
1.6 meV/Mn
0.7 meV/Mn
E-E_F (eV)
K ← Γ → M
(f) (g) (h) (i) (j)
-X ← Γ → X
AFM
FM
I
II
III

Axion mass



It can be suppressed near the phase boundary

Rich magnetic topological states in that region?