Spin Berry phase in topological insulators and Weyl semimetals

Ken Imura
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in collaboration with

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(Hiroshima) (NIMS)

Spin Berry phase in gapped and gapless topological phases

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Spin-to-surface locking in gapped and gapless topological phase

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- Gapped vs. gapless topological phases:

d=3

topological insulators → Gapped
weak & strong

Weyl semimetal → gapless

bulk: topological invariants
surface: (protected) gapless surface states

- Specific types of *protected* surface states:

  1. helical: Dirac cone(s) ← topological insulators

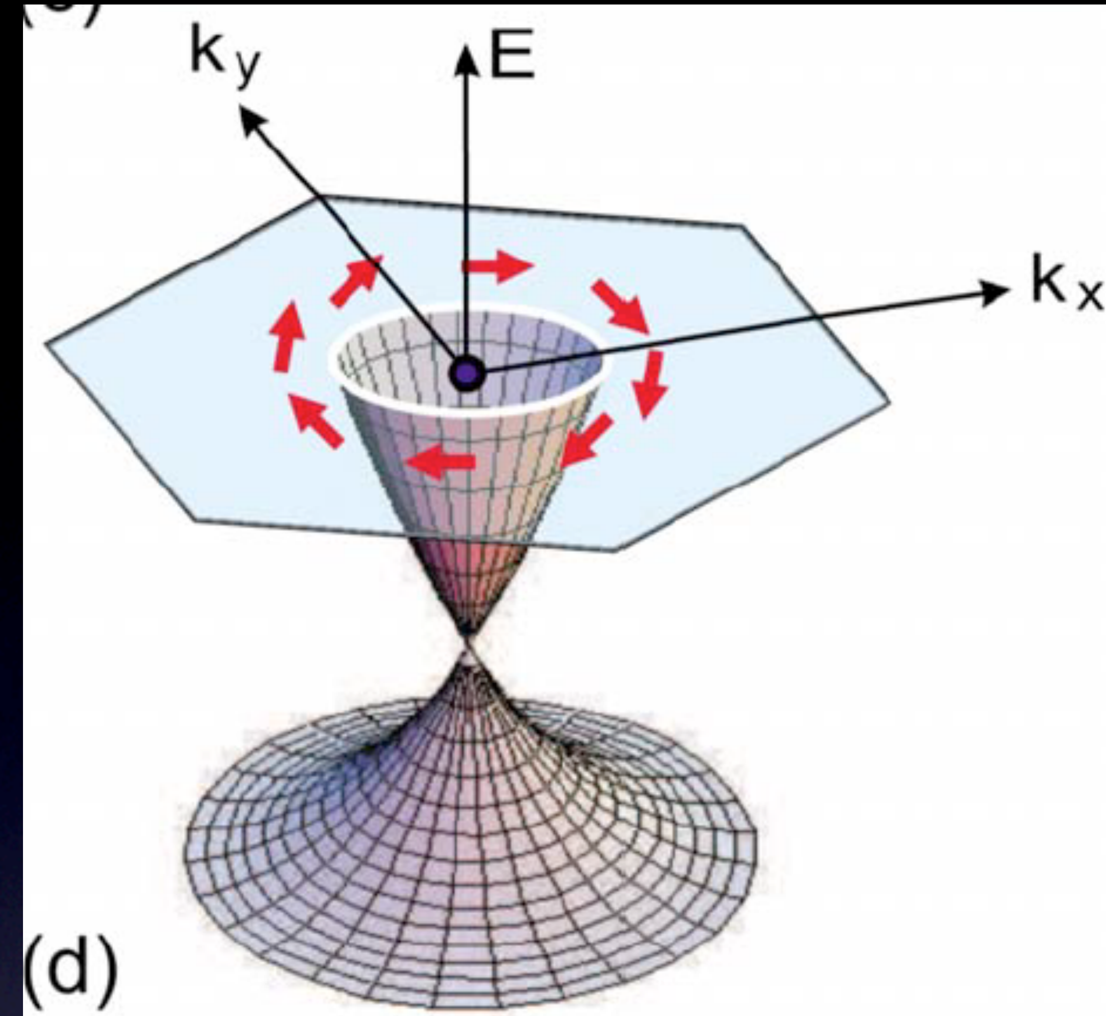
  2. chiral: Fermi arc states ← Weyl semimetal

- Highlight on the "*spin-to-surface* locking"

  → *spin Berry phase*

What is the spin-to-surface locking?

Not this one.



This is often referred to as "*spin-to-momentum*" locking

Hasan & Kane, Rev. Mod Phys. '10

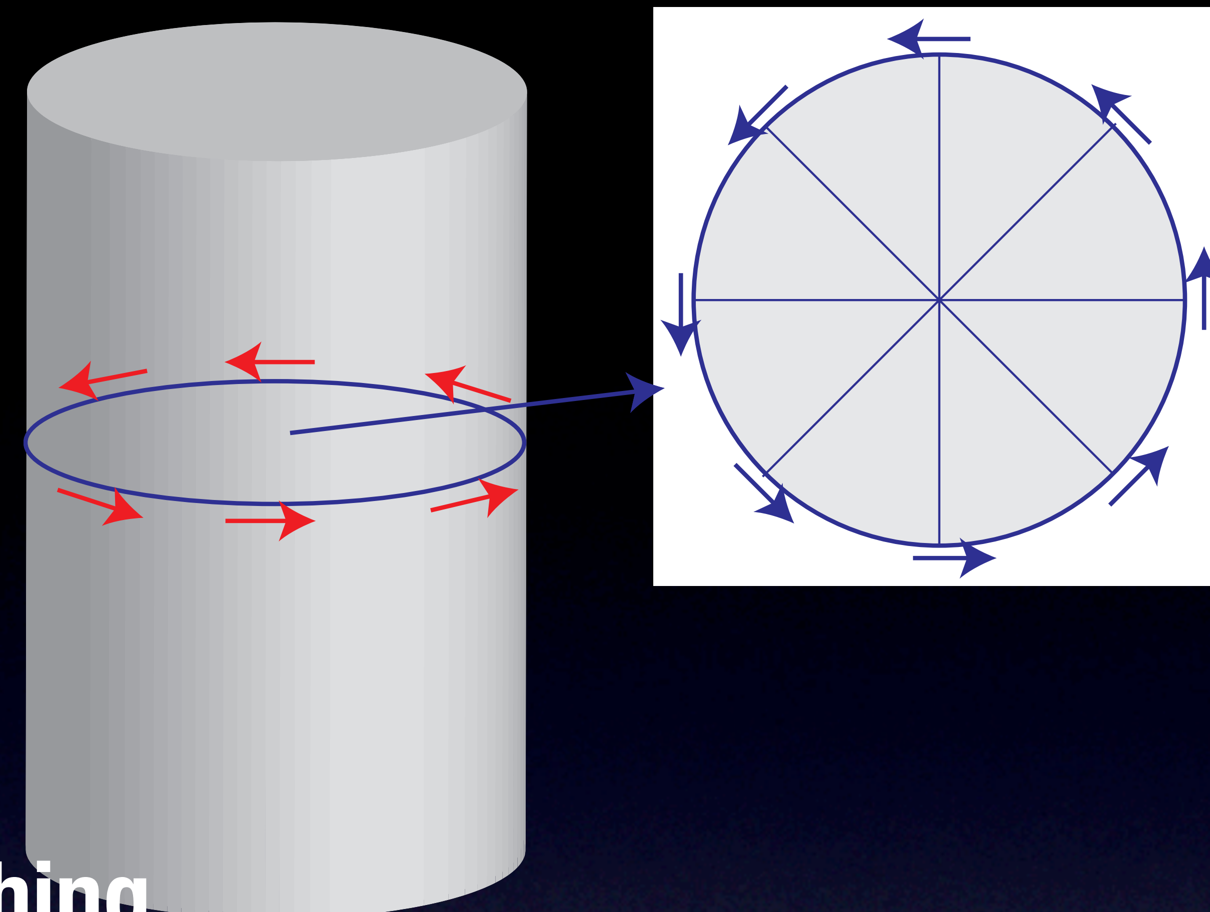
Figure 1 | Detection of spin-momentum locking of spin-helical Dirac electrons in Bi_2Se_3 and Bi_2Te_3 using spin-resolved ARPES. a, b, ARI

Hsieh et al., Nature, '09

The surface effective Hamiltonian:

$$H_{2D} = A(\boldsymbol{\sigma} \times \boldsymbol{k})_z$$

Zhang et al. Nature Phys. '10; Liu et al., PRB '10, Shan et al. NJP '10 so far everything was on a ***flat*** surface



What happens?

if one repeats the same procedure on a ***curved*** surface (cylinder)

Ans.: One finds almost the same thing.

$$H_{2D} = A \begin{bmatrix} 0 & -ik_z + \frac{1}{R}\left(-i\frac{\partial}{\partial\phi} + \frac{1}{2}\right) \\ ik_z + \frac{1}{R}\left(-i\frac{\partial}{\partial\phi} + \frac{1}{2}\right) & 0 \end{bmatrix}$$

KI, Takane & Tanaka, Phys. Rev. B 84, 195406 (2011)

but with one important correction: the “spin Berry phase”

Zhang & Vishwanath PRL ’10; Ostrovsky et al., PRL ’10, Bardarson et al. PRL ’10, ...

Interpretation: the “spin-to-surface” locking

spin = locked ***in-plane*** to the surface, i.e.,

with its frames following the tangential plane of the curved surface *plan of the talk*

part 1

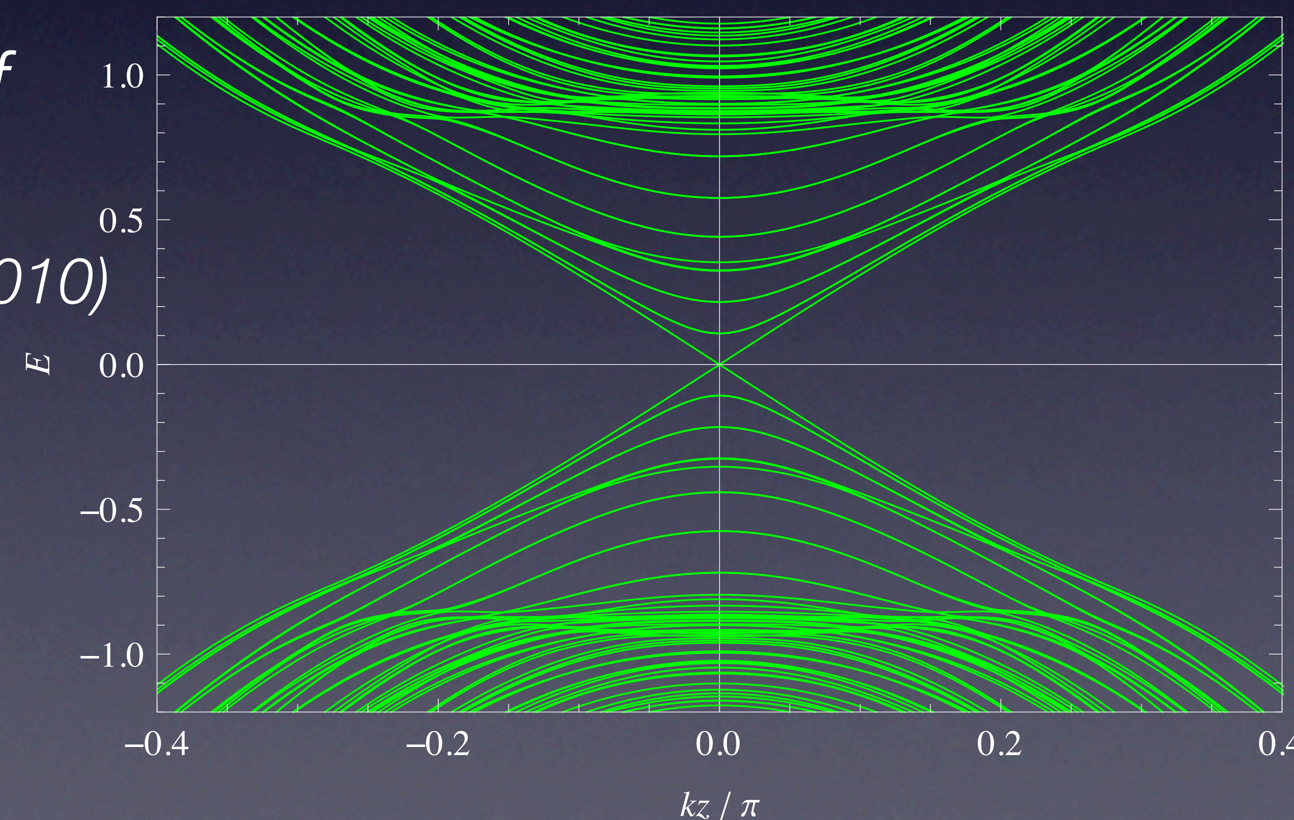
0) spin Berry phase: a brief sketch of its derivation

1) spin-to-surface locking in topological insulators

- direct consequences of the spin-to-surface locking:
  1. ***Half-integer*** quantization of the ***orbital*** angular momentum
  2. Enhancement of finite-size corrections:
     ΔE decays only ***algebraically***

relevance to the classification of topological defects in

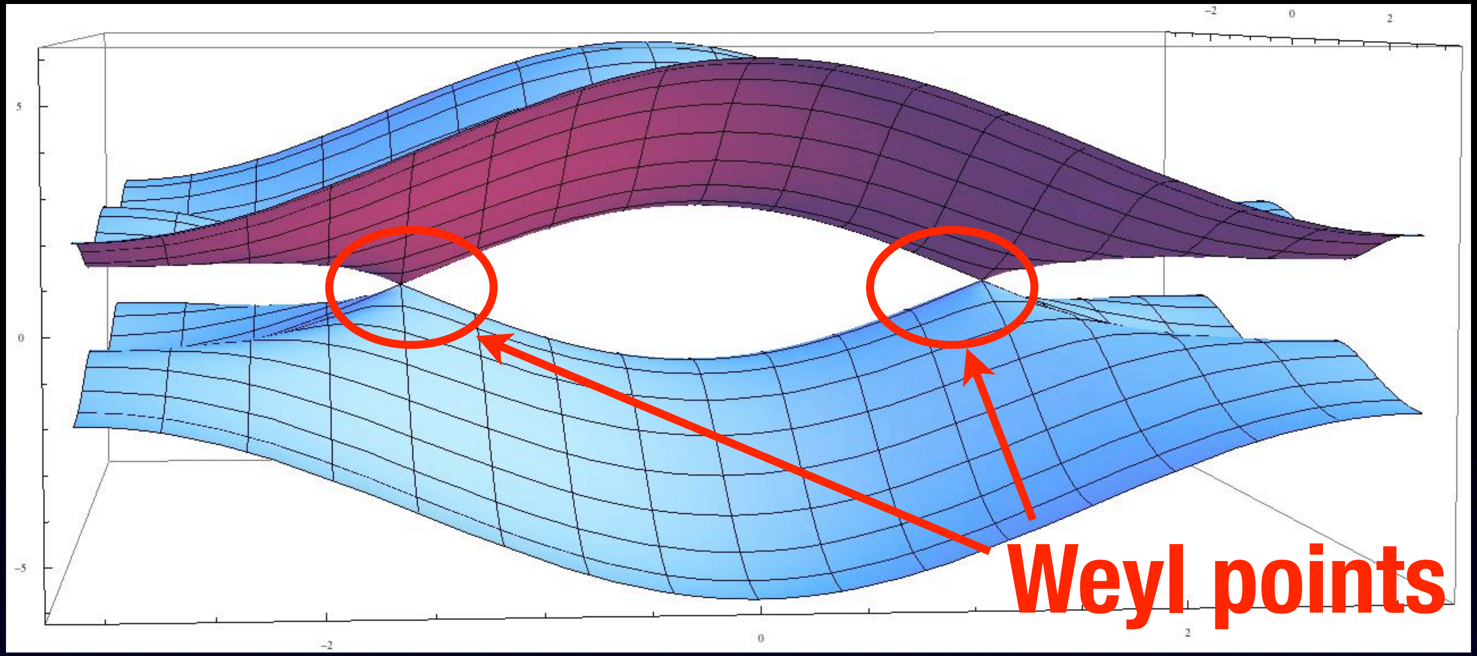
Teo & Kane, Phys. Rev. B 82, 115120 (2010)

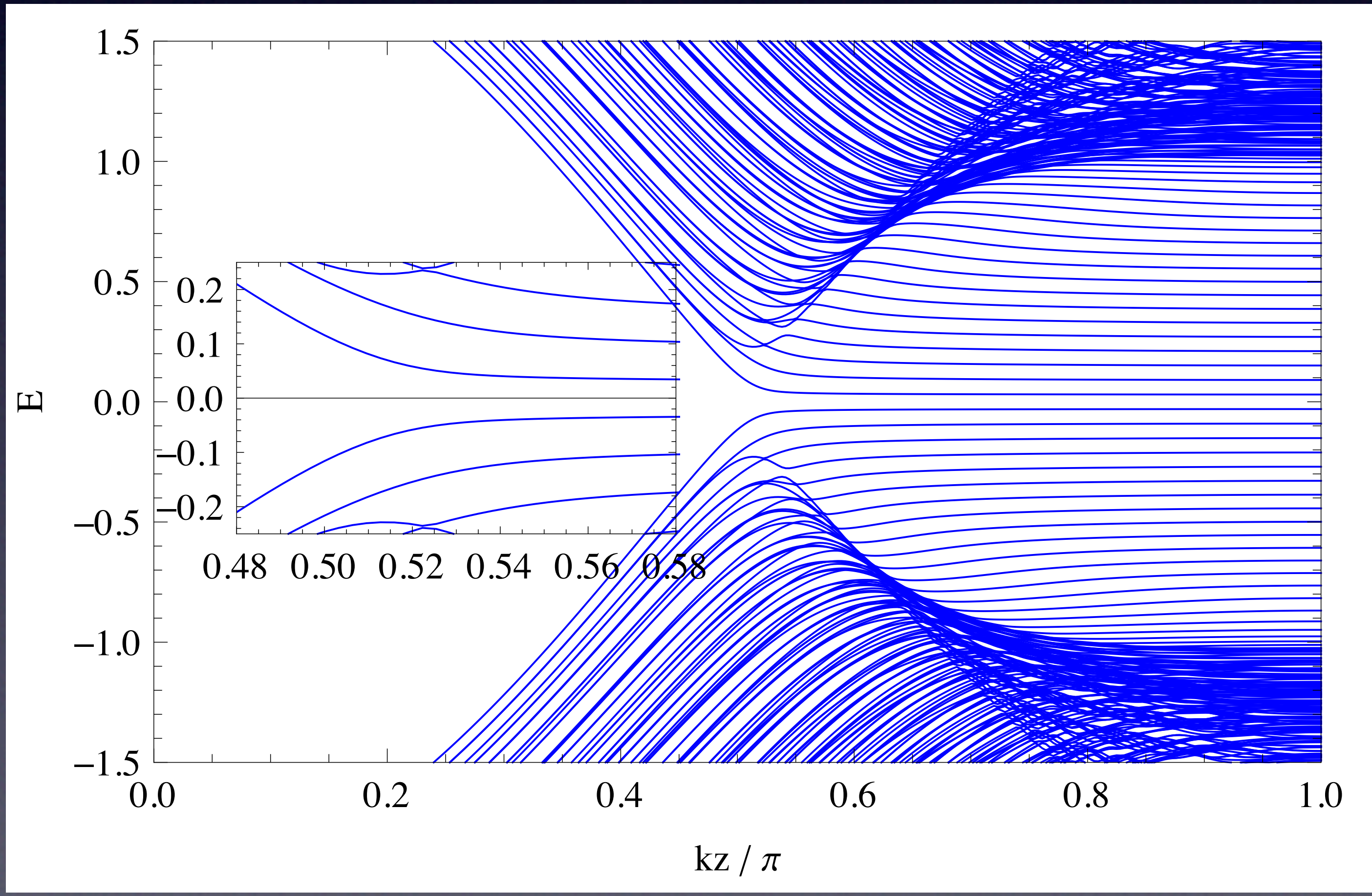


- further applications:
  e.g., 1D ***gapless*** helical modes, associated with
  i) a pi-flux tube
  ii) dislocation lines

part 2

2) Characteristic feature of the spin-to-surface locking in the Fermi arc surface states of a Weyl semimetal





- ***chiral*** spin-to-surface locking
- completely ***flat*** multiple subbands
- flatness: topologically protected

KI & Takane, arXiv:1109.3234, Phys. Rev. B in press.

The spin Berry phase: sketch of its derivation

- starting with a 3D bulk effective Hamiltonian:

$$H_{3D} = A(p_x\gamma_1 + p_y\gamma_2 + p_z\gamma_3) + m\gamma_0$$

$$\{\gamma_i, \gamma_j\} = 2\delta_{ij} \qquad m(\boldsymbol{p}) = m_0 + m_2\boldsymbol{p}^2$$

- Having in mind that we will consider a boundary value problem of this sort, →

$$|\psi\rangle_{r=R} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

we decompose the Hamiltonian into two parts:

$$H = H_\perp(k_r) + H_\parallel(k_\phi, k_z)$$

$$r = \sqrt{x^2 + y^2} \qquad \phi = \arctan\frac{y}{x}$$

- First, find in-gap surface solutions of the radial eigenvalue problem:

$$H_\perp|\psi\rangle = E_\perp|\psi\rangle \qquad |\psi\rangle \sim e^{\lambda(r-R)}$$

- Then, find a linear combination: $|\psi\rangle = \sum_{j=1}^{4} c_j |\psi_j\rangle$

  that is compatible with the boundary condition: $|\psi\rangle_{r=R} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

  which turns out to be $E_\perp = 0$

$$|\psi\rangle = \left[\frac{c_1}{2} \begin{bmatrix} 1 \\ i \\ e^{i\phi} \\ ie^{i\phi} \end{bmatrix} + \frac{c_2}{2} \begin{bmatrix} 1 \\ -i \\ -e^{i\phi} \\ ie^{i\phi} \end{bmatrix} \right] \rho(r)$$

$$\equiv c_1 |\boldsymbol{r}+\rangle\rangle + c_2 |\boldsymbol{r}-\rangle\rangle$$

$$|\hat{\boldsymbol{r}}+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ e^{i\phi} \end{bmatrix}$$

$$|\hat{\boldsymbol{r}}-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -e^{i\phi} \end{bmatrix}$$

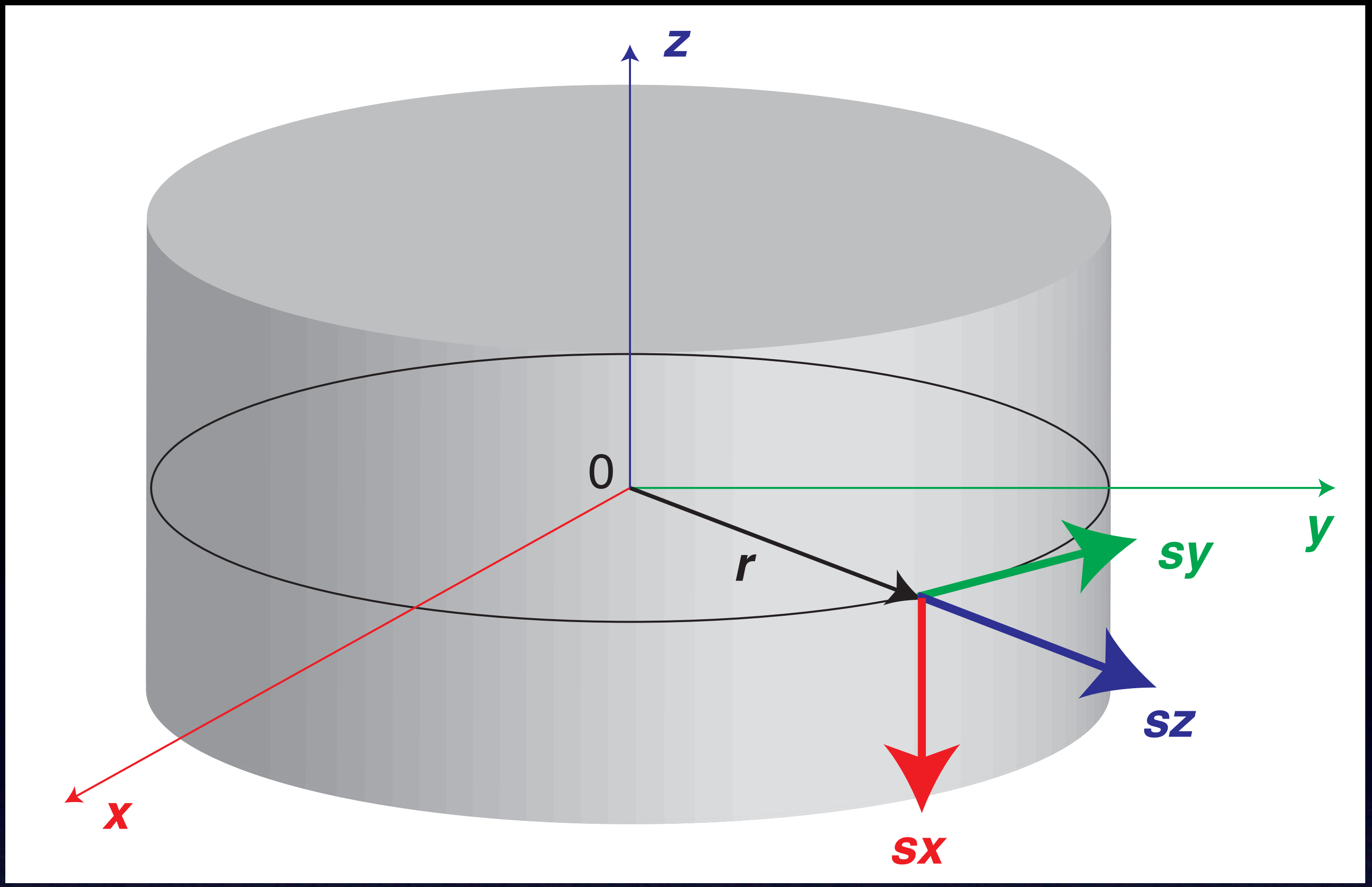
- Calculating the matrix elements: $(H_{2D})_{\pm\pm} = \langle\langle \boldsymbol{r} \pm | H_{\parallel} | \boldsymbol{r} \pm \rangle\rangle$

  one finds

$$H_{2D} = A \begin{bmatrix} 0 & -ik_z + \frac{1}{R}\left(-i\frac{\partial}{\partial\phi} + \frac{1}{2}\right) \\ ik_z + \frac{1}{R}\left(-i\frac{\partial}{\partial\phi} + \frac{1}{2}\right) & 0 \end{bmatrix}$$

The “spin Berry phase”

Interpretation of the factor 1/2: the "spin-to-surface locking"



- possible to ***absorb*** the 1/2 factor in the definition of the (c1,c2)-spinor:

$$H_{2D}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E_{\|}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = e^{-i\phi/2}\begin{bmatrix} \chi_1 \\ \chi_2 \end{bmatrix} \qquad \boldsymbol{\chi} = \frac{1}{\sqrt{2}}\begin{bmatrix} e^{-i\eta/2} \\ \pm e^{i\eta/2} \end{bmatrix}$$

- In the ***transformed*** basis, with some ***redefinition*** of the spin frame, one can rewrite the surface effective Hamiltonian as

$$\hat{\boldsymbol{s}}_x : \quad \hat{\boldsymbol{x}} \longrightarrow -\hat{\boldsymbol{z}}$$
$$\hat{\boldsymbol{s}}_y : \quad \hat{\boldsymbol{y}} \longrightarrow \hat{\boldsymbol{\phi}}$$
$$\hat{\boldsymbol{s}}_z : \quad \hat{\boldsymbol{z}} \longrightarrow \hat{\boldsymbol{r}}$$

$$H_{2D}^{(\boldsymbol{\chi})} = A\sigma_x k_\phi + B\sigma_y k_z$$
$$\sim A(\boldsymbol{\sigma} \times \boldsymbol{k})_z$$

M*anifestations*
of the spin Berry phase

in weak and strong topological insulators

- ***Half-integer*** quantization of the orbital angular momentum
- Finite-size energy gap: ***algebraic*** decay
- 1D ***gapless*** helical modes, associated with

i) a pi-flux tube ii) dislocation lines

A direct consequence of the spin Berry phase:

Half-integer quantization of the *orbital* angular momentum

radius: R

Electronic state on the surface of a ***cylinder***

- orbital part: plane-wave like

$$H_{2D}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E_{\parallel}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$$\psi(\phi, z) = e^{i(p_\phi R\phi + p_z z)}$$

$$E_{\parallel} = \pm A\sqrt{p_\phi^2 + p_z^2}$$

- boundary condition: periodic → anti-periodic

$$e^{iL_z(\phi+2\pi)} \times \underline{(-1)} = e^{iL_z\phi} \qquad L_z = p_\phi R$$

spin Berry phase

$$L_z = \pm 1/2, \pm 3/2, \cdots$$

(half-integer quantization)

→ gap opening

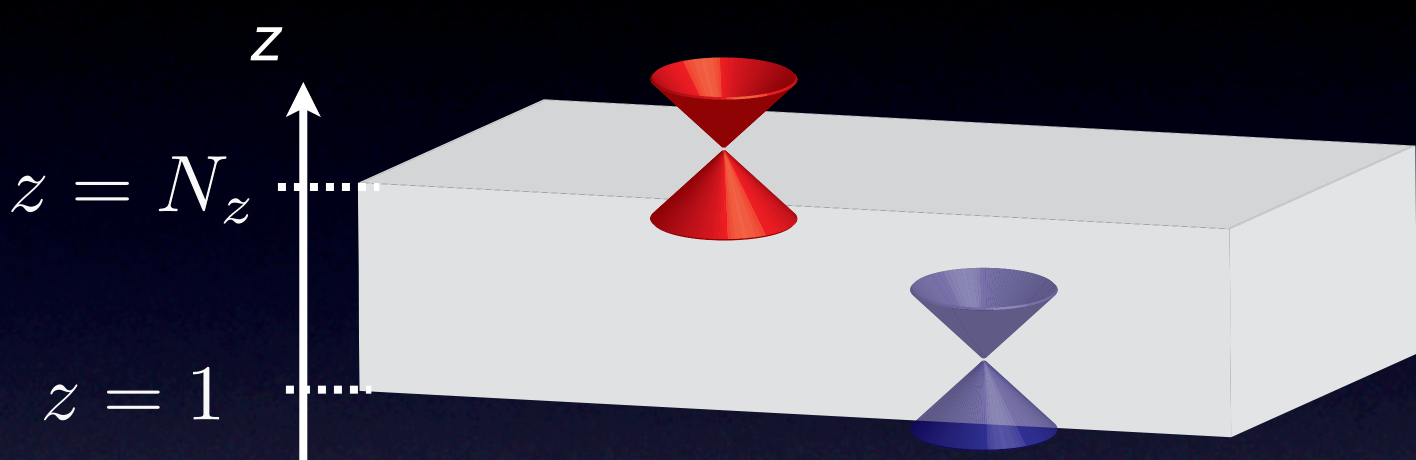
$$\Delta E = A/R \propto R^{-1}$$

→ ***algebraic*** decay of the finite-size energy gap

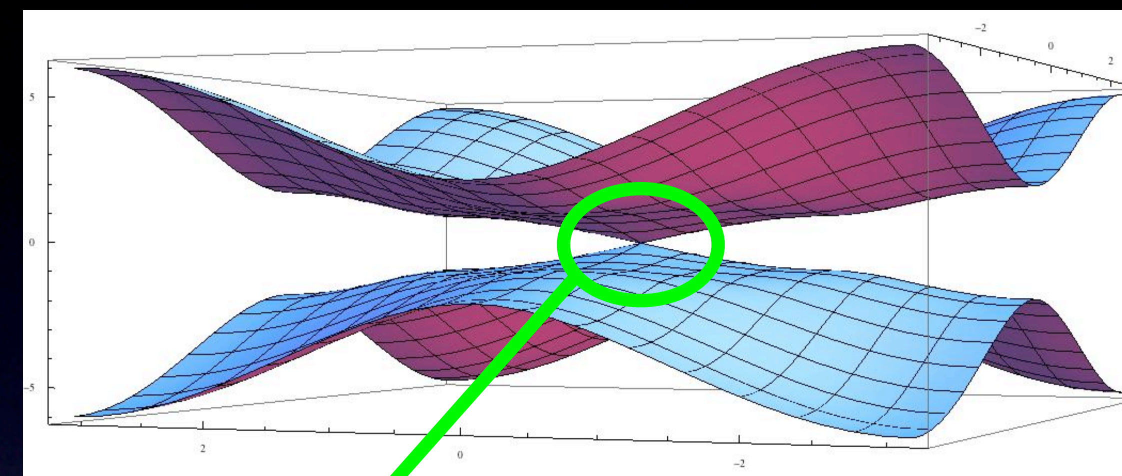
(strong finite-size effects)

Finite-size energy gap: ***algebraic*** decay

- conventional finite-size energy gap: exponential decay

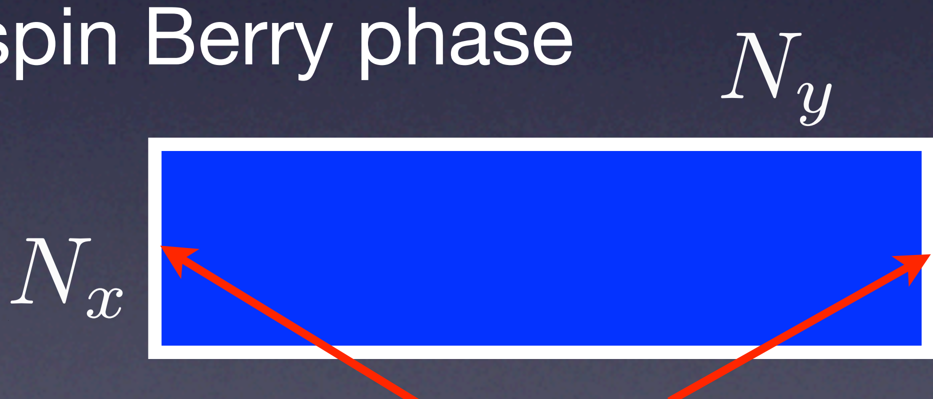


infinitely large slab (thin film) of a TI



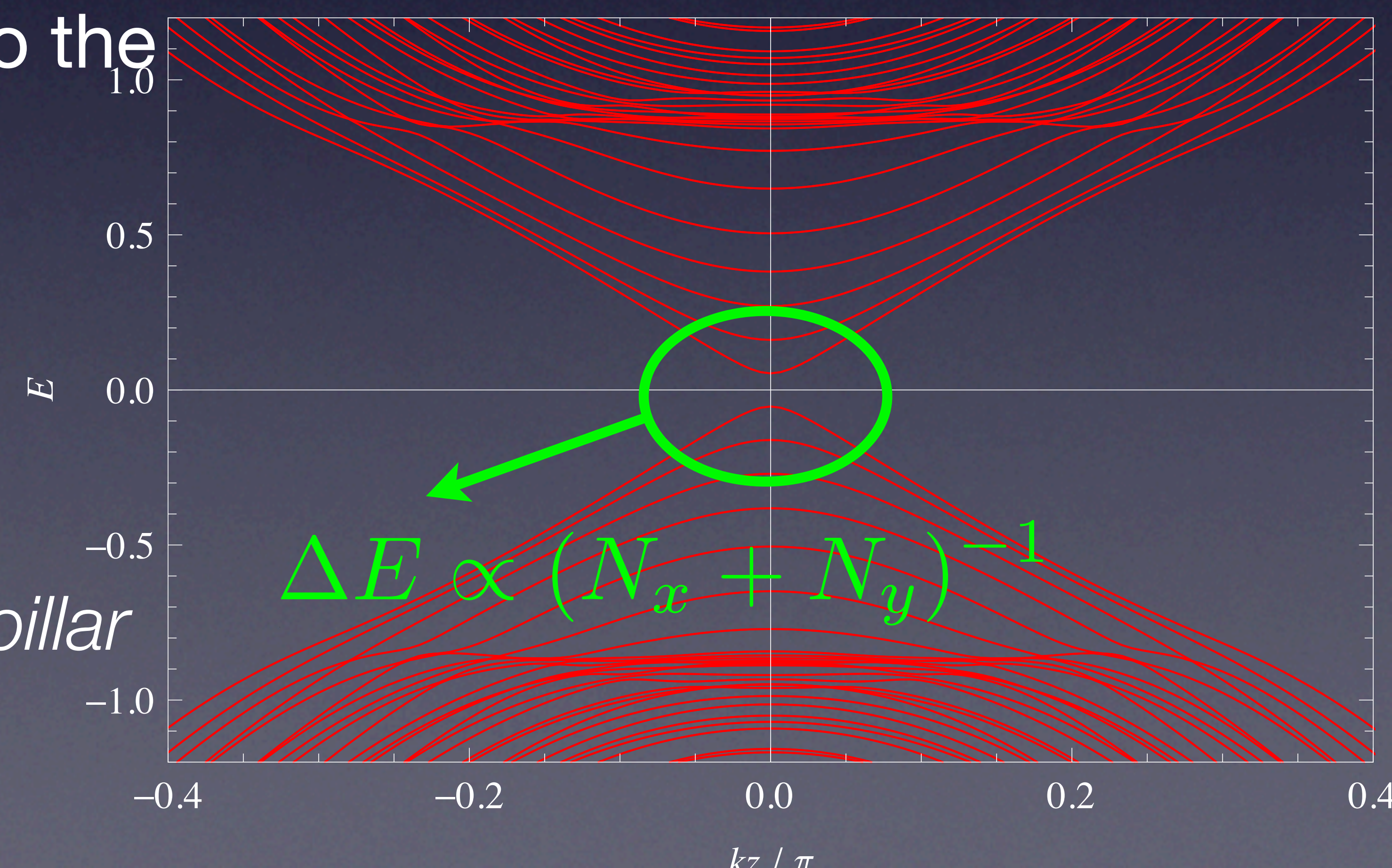
$$\Delta E \propto e^{-\alpha N_z}$$

- finite-size energy gap due to the spin Berry phase



slab with ***two side surfaces***

= an (infinitely long) rectangular pillar



$$\Delta E \propto (N_x + N_y)^{-1}$$

1D gapless helical modes

associated with i) a pi-flux tube

- First recall the ***half-integer*** quantization:

$$e^{iL_z(\phi+2\pi)} \times \underline{(-1)} = e^{iL_z\phi}$$ ⟵ *anti-p.b.c*

spin Berry phase

$$L_z = \pm 1/2, \pm 3/2, \cdots$$

- In the presence of an Aharonov-Bohm flux tube, this modifies as

$$e^{iL_z(\phi+2\pi)} \times \underline{e^{i\Phi_{AB}}} \times \underline{(-1)} = e^{iL_z\phi}$$

AB flux

$$E = \pm A\sqrt{p_\phi^2 + p_z^2}$$

$$L_z = p_\phi R$$

IF the AB flux: $\Phi/\pi = \pm 1, \pm 3, \pm 5, \cdots$

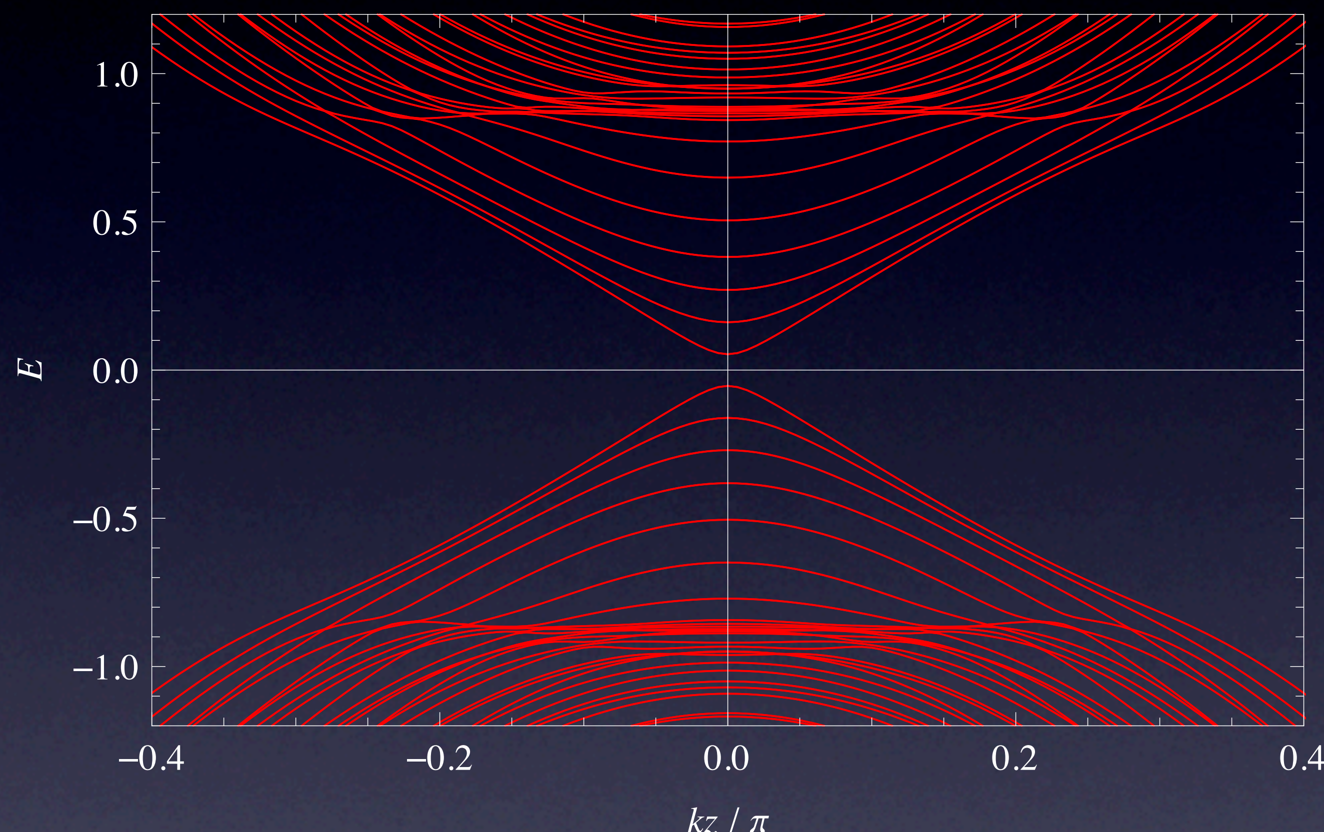
THEN, $L_z = \underline{0,} \pm 1, \pm 2, \cdots$

gapless

Energy spectrum of a rectangular pillar of TI

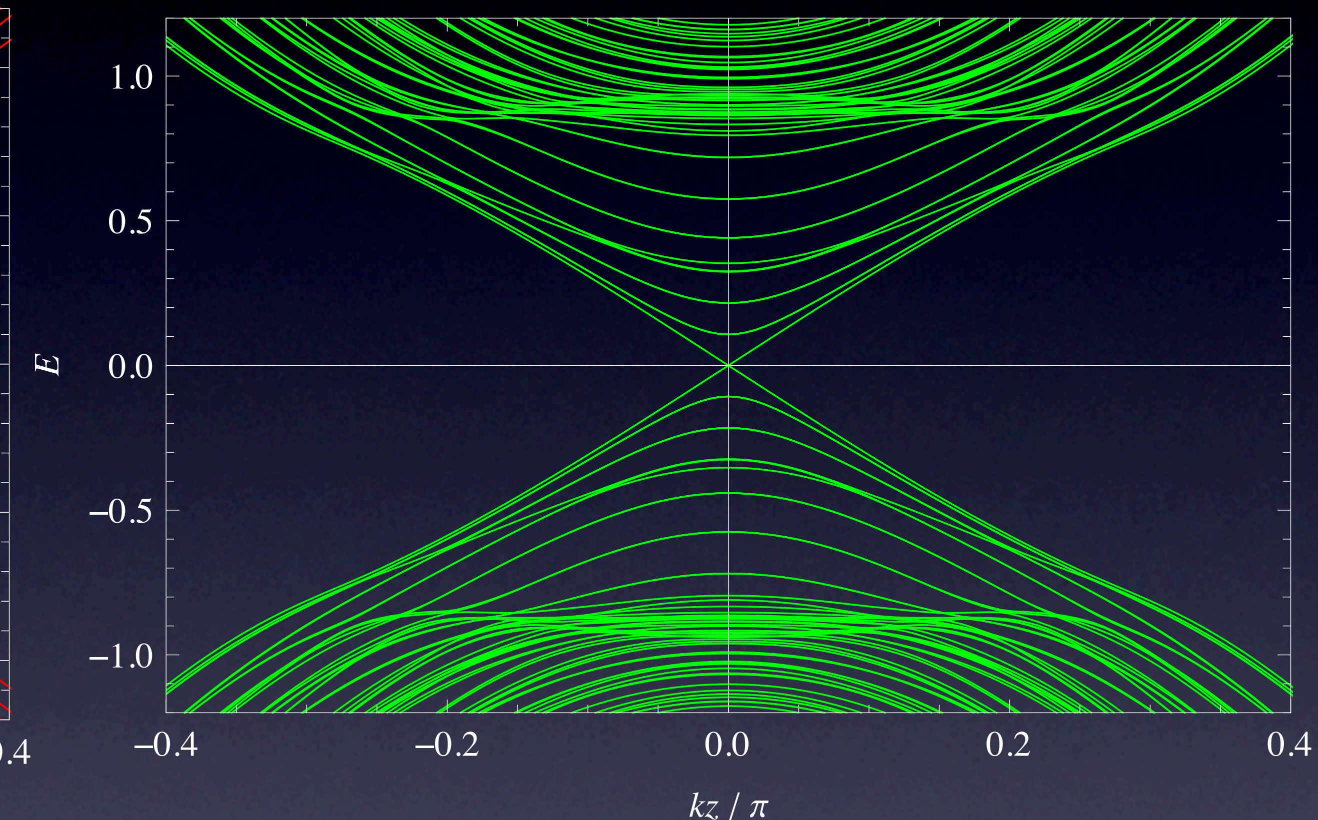
- In the ***absence*** of AB flux

$$\Phi_{AB} = 0$$



- In the ***presence*** of AB flux

$$\Phi_{AB} = \pi$$



spin Berry phase π

→ *anti-p.b.c*

→ spectrum: gapped

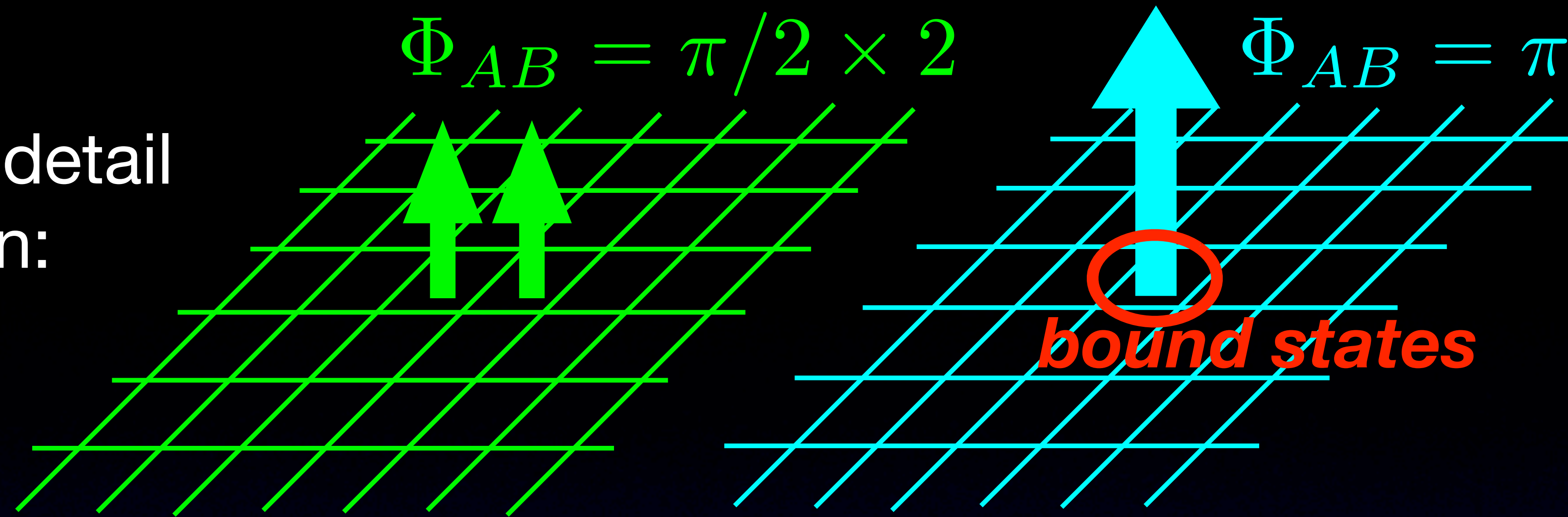
spin Berry phase & AB flux

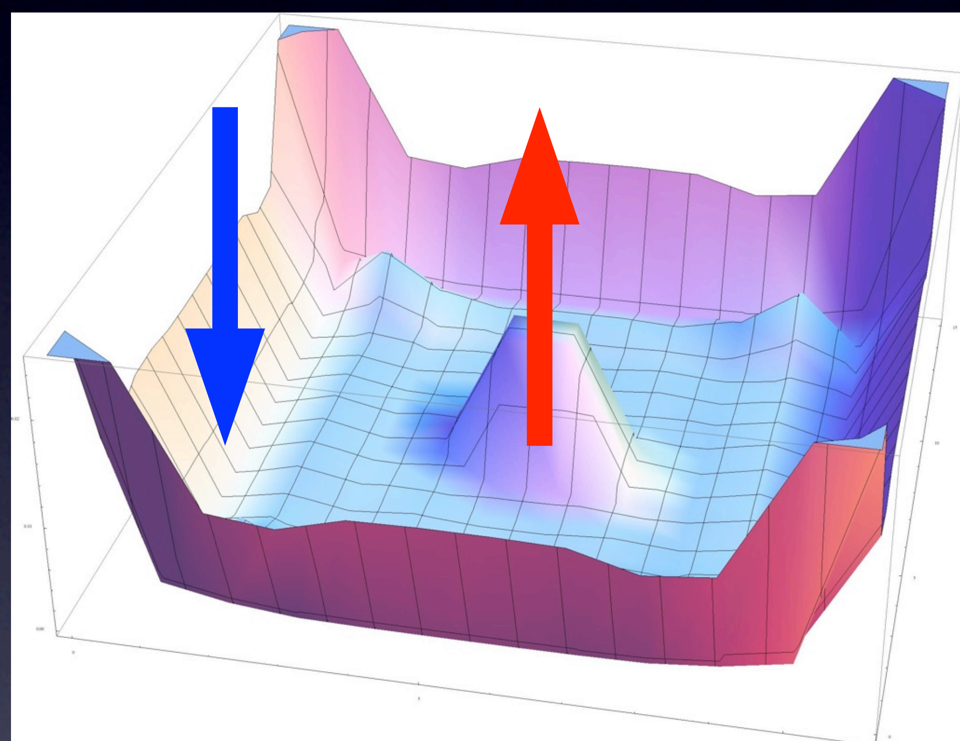
$$\pi + \pi = 2\pi \simeq 0$$

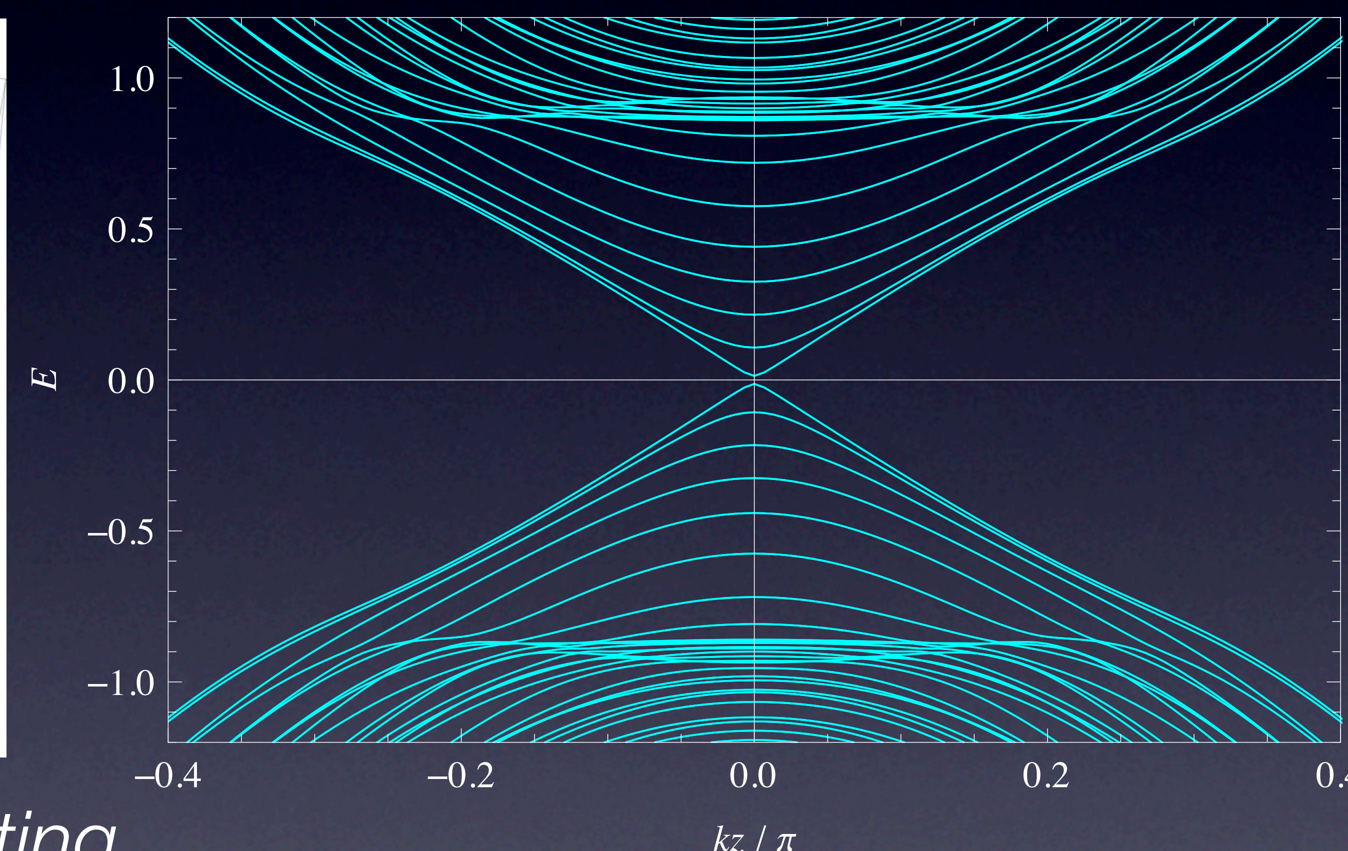
→ gapless

Zhang & Vishwanath PRL '10; Ostrovsky et al., PRL '10, Bardarson et al. PRL '10, ...

An important (?) detail of this calculation:







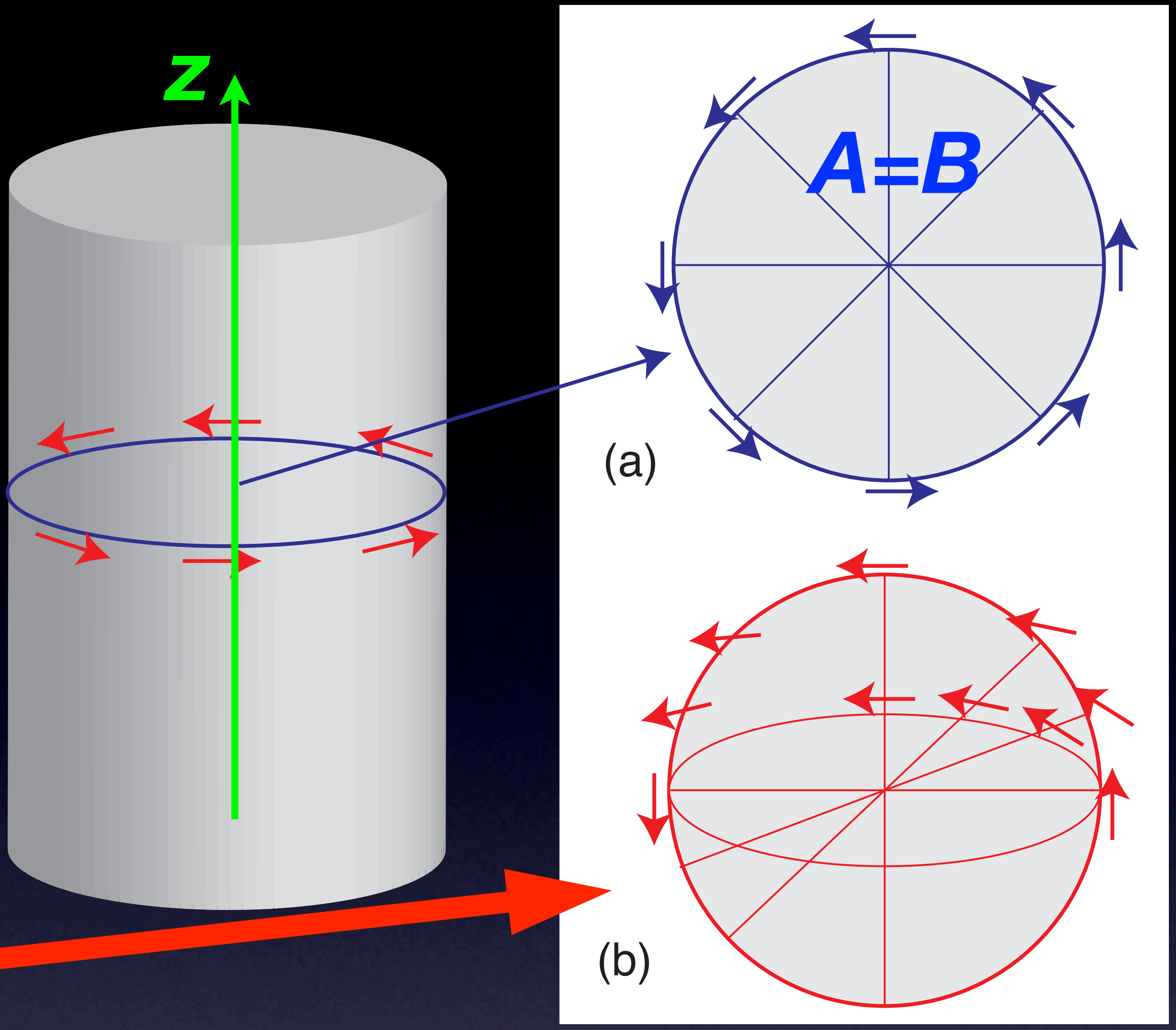
mixing of counter-propagating 1D modes → gapped spectrum

pi-flux piercing a plaquette ⟷ bound states

KI, Takane & Tanaka, Phys. Rev. B 84, 195406 (2011)

A remark on the ***anisotropic*** case

(a remark for the experts)



- <u>anisotropy</u> associated with the crystal growth axis
- Spin-to-surface locking is ***not a local concept !***
- Only the ***global*** π-phase shift is robust.

$$A \neq B$$

$$H_{3D} = M\tau_z + \tau_x(B\sigma_x k_x + A\sigma_y k_y + A\sigma_z k_z)$$

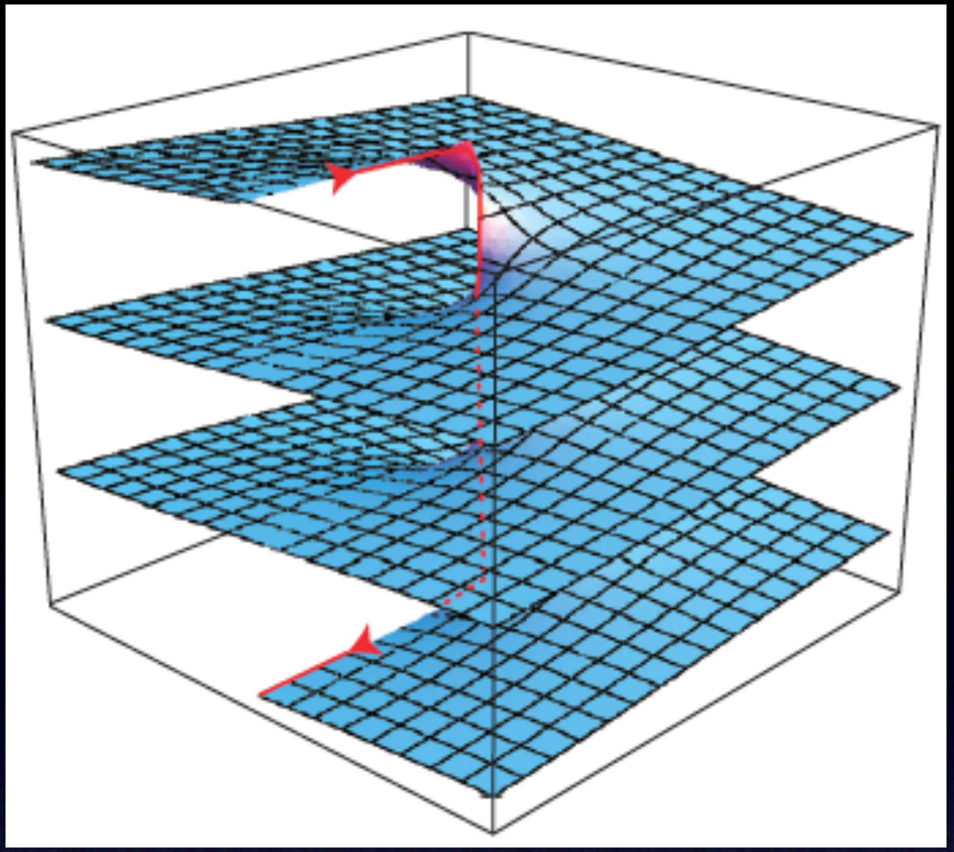
anisotropy along the x-axis

KI, Takane & Tanaka, Phys. Rev. B 84, 195406 (2011)

1D gapless helical modes

associated with

ii) dislocation lines



Ran, Zhang & Vishwanath, Nature Physics, 5, 298 (2009)

- First recall the ***half-integer*** quantization:

$$e^{iL_z(\phi+2\pi)} \times \underline{(-1)} = e^{iL_z\phi}$$

spin Berry phase

$$L_z = \pm 1/2, \pm 3/2, \cdots$$

- In the presence of a screw dislocation, this modifies as

$$e^{iL_z(\phi+2\pi)} \times \underline{e^{ik_z^{(0)}b}} \times \underline{(-1)} = e^{iL_z\phi}$$

screw dislocation

Burgers vector:

$$\boldsymbol{b} = (0, 0, b)$$

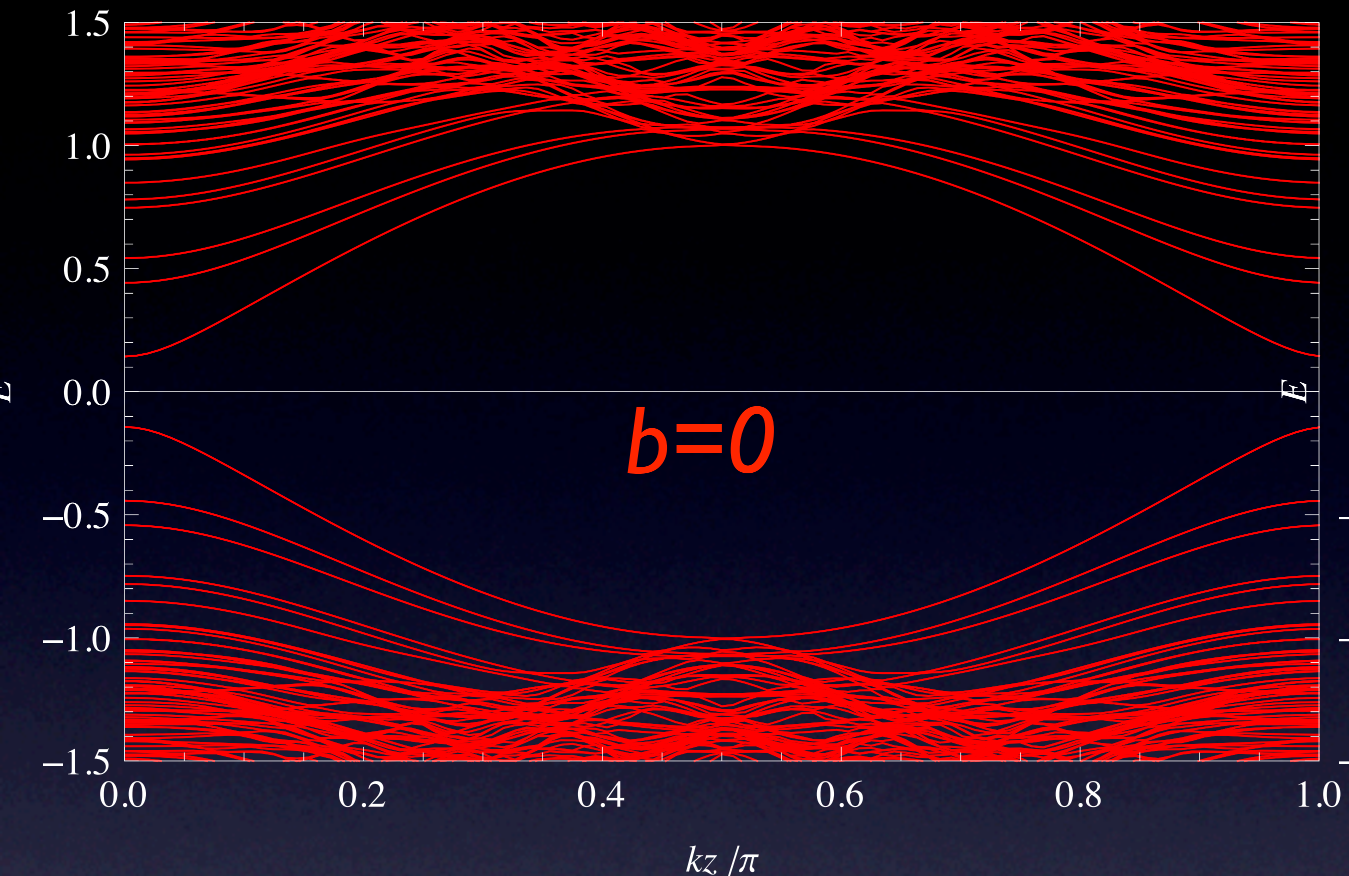
IF $k_z^{(0)} = \pi$ **AND** *b=1,3,5,...* → even/odd feature w.r.t. ***b***

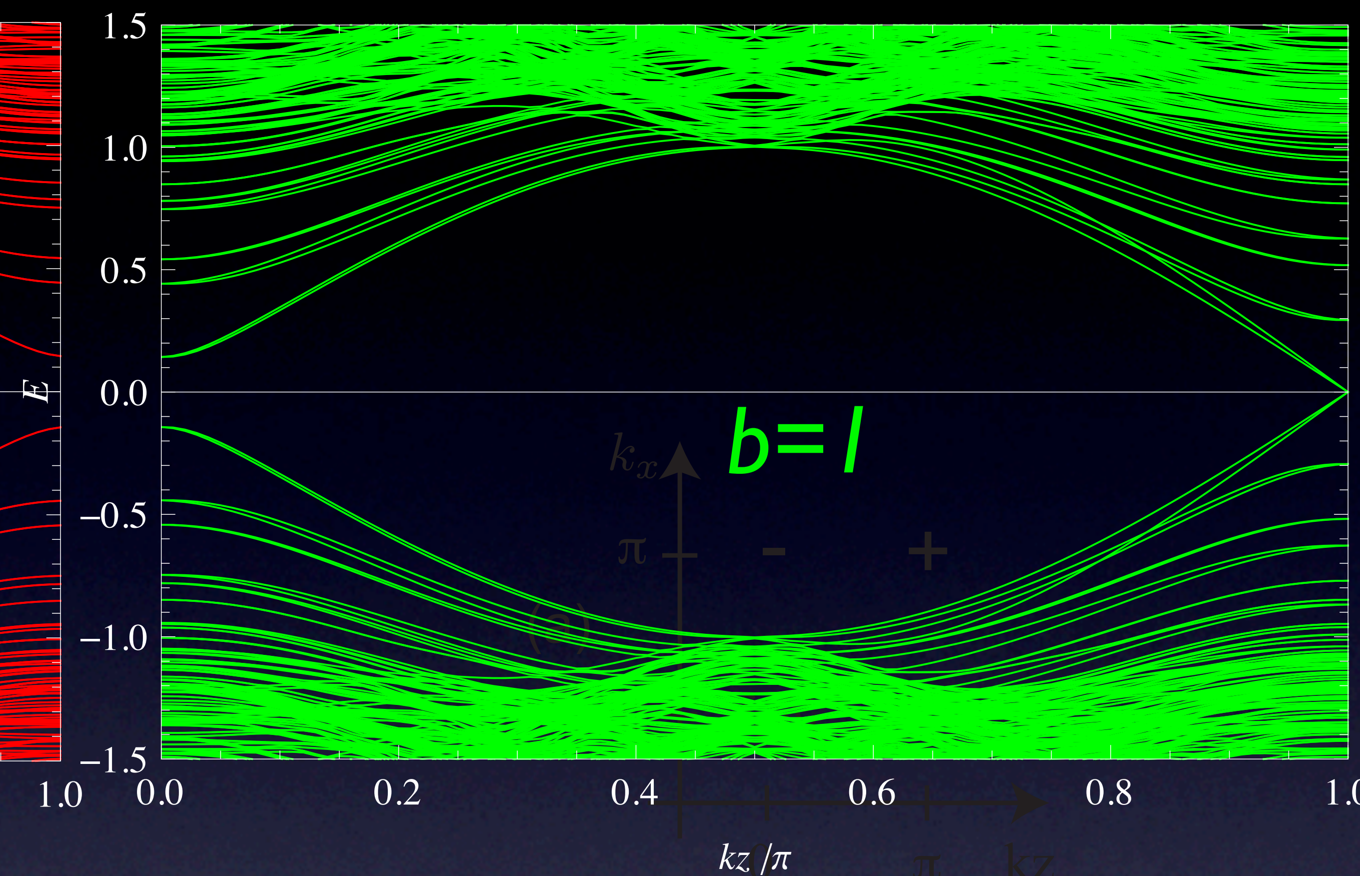
THEN, $L_z = \underline{0}, \pm 1, \pm 2, \cdots$

gapless

KI, Takane & Tanaka, Phys. Rev. B 84, 035443 (2011)

Even/odd feature with respect to b



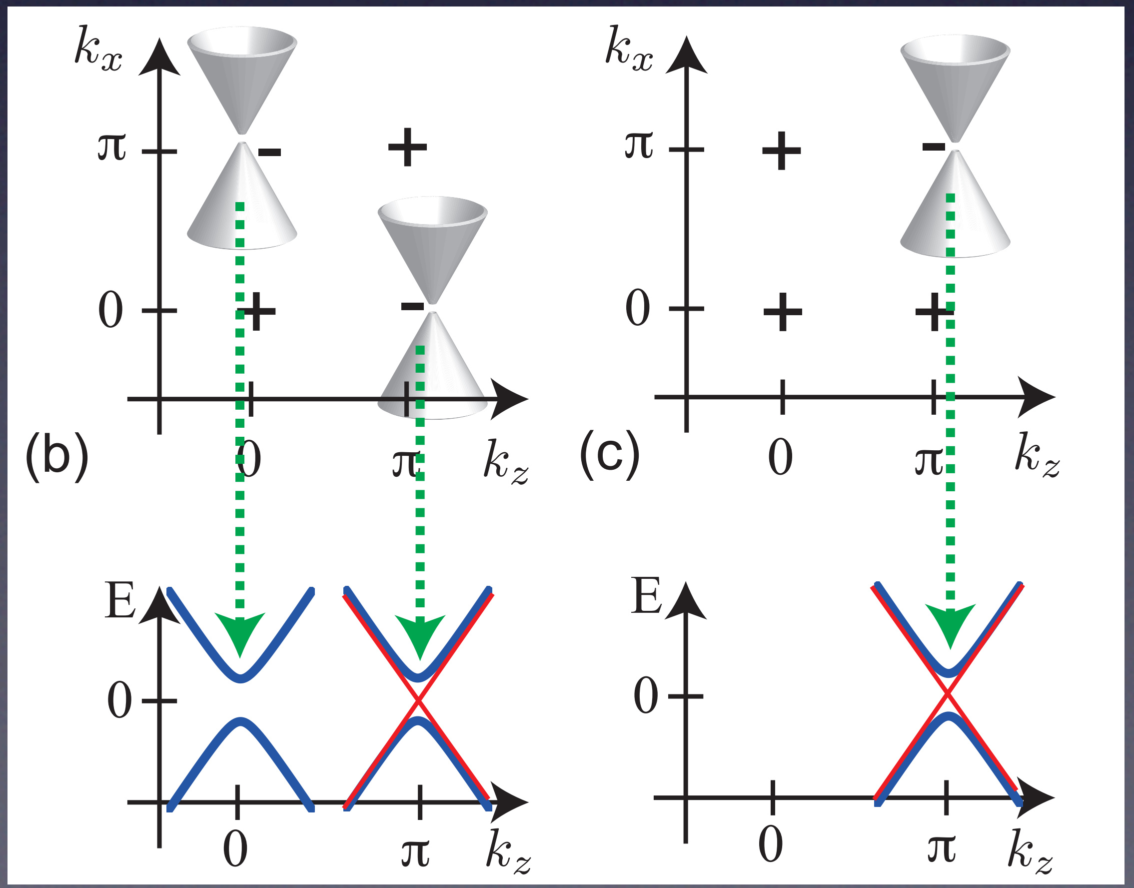


- ***The Dirac cone at***

$$k_z^{(0)} = \pi$$

susceptible of the screw dislocation with

$$\boldsymbol{b} = (0, 0, b)$$



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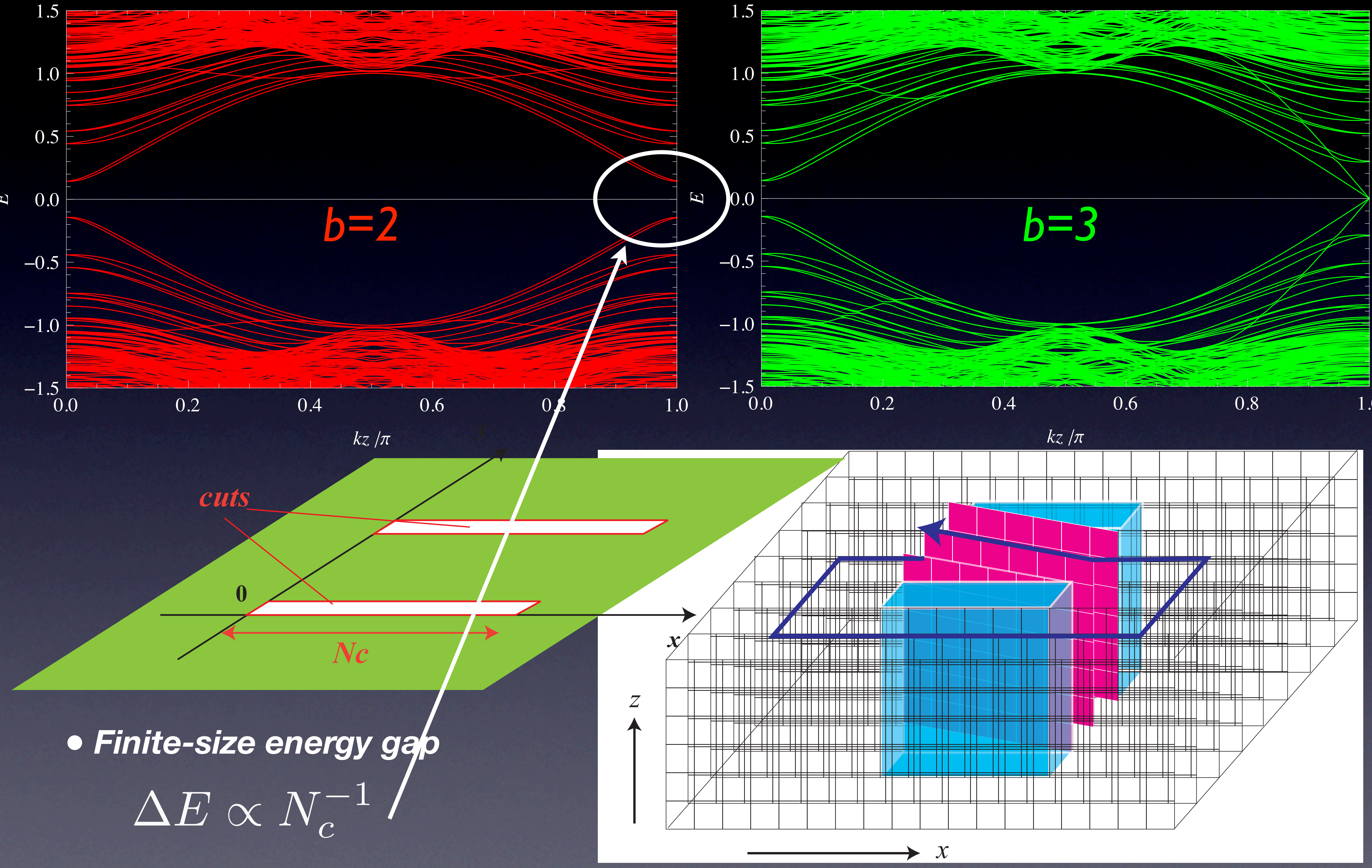


- ***Finite-size energy gap***

$$\Delta E \propto N_c^{-1}$$

KI, Takane & Tanaka, Phys. Rev. B 84, 035443 (2011)

some remarks

- role of ***weak indices:***

condition for the existence of such 1D gapless helical modes

$$\vec{M} \cdot \vec{b} = \pi \mod 2\pi \qquad \vec{M} = \frac{1}{2}(\nu_1 \vec{G}_1 + \nu_2 \vec{G}_2 + \nu_3 \vec{G}_3)$$

Ran, Zhang & Vishwanath, Nature Physics, 5, 298 (2009)

- 1D gapless helical modes ***protected by the finite-size energy gap***

KI, Takane & Tanaka, Phys. Rev. B 84, 035443 (2011)

Summary of the 1st half of talk

1. The spin-to-surface locking

   i) leads to the ***half-integer*** quantization of the ***orbital*** angular momentum
   ii) is ***not a local*** concept

2. Further manifestations of the spin-to-surface locking:

   i) strong finite-size effects in ***TI nanowires***
   ii) 1D gapless helical modes along a ***pi-flux tube*** and ***dislocation lines***

KI, Takane & Tanaka, Phys. Rev. B 84, 195406 (2011)
KI, Takane & Tanaka, Phys. Rev. B 84, 035443 (2011)

- Aharonov-Bohm measurement in TI nanowires

Peng et al., Nature Materials 9, 225 (2010) *part 2*

How about the case of gapless topological phases?

- **3D Weyl semimetal may be realized in pyrochlore iridates: A2Ir2O7**

L. Balents, Physics '11

X. Wan et al. PRB '11; W. Witczak-Krempa & Y.-B. Kim, arXiv:1105.6108, ...

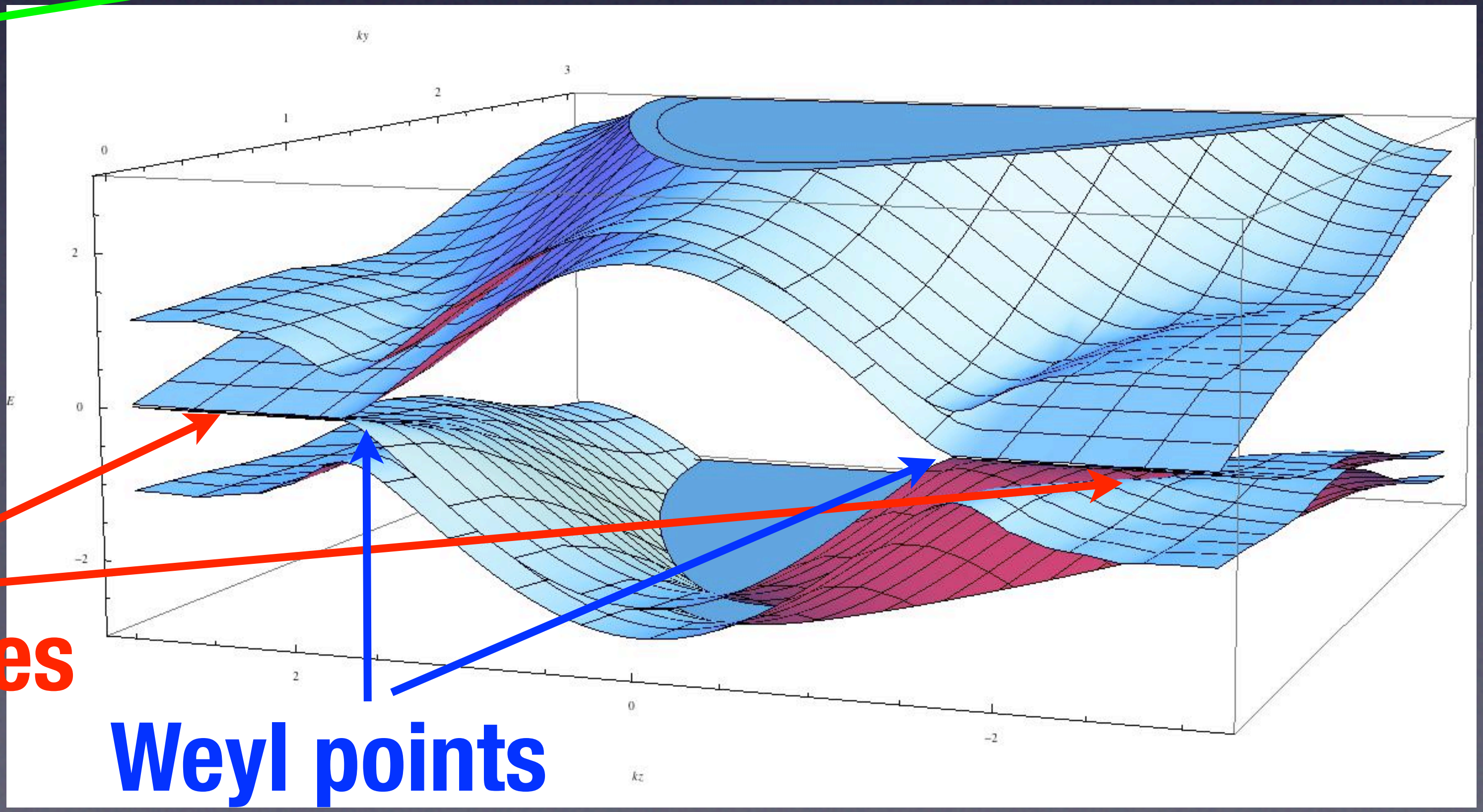
or maybe somewhere else, in some other formats...

A.A. Burkov & L. Balents, arXiv:1105.5138, G. Xu et al. arXiv:1106.3125,...

- **3D Weyl semimetal is a 3D version of graphene:**

flat edge modes of graphene (zigzag, bearded edges)	→	**Fermi arc states**
2D		**3D**

surface states of topological origin



Fermi arc states

Weyl points

Classification of the gapless topological phases

A. Schnyder, KITP, 2011;
G.E. Volovik, books

2D example

- **graphene**
- **class AIII**
- **protected point node : Z-type**

$$H(\boldsymbol{k}) = \begin{bmatrix} 0 & f(\boldsymbol{k}) \\ f^*(\boldsymbol{k}) & 0 \end{bmatrix}$$

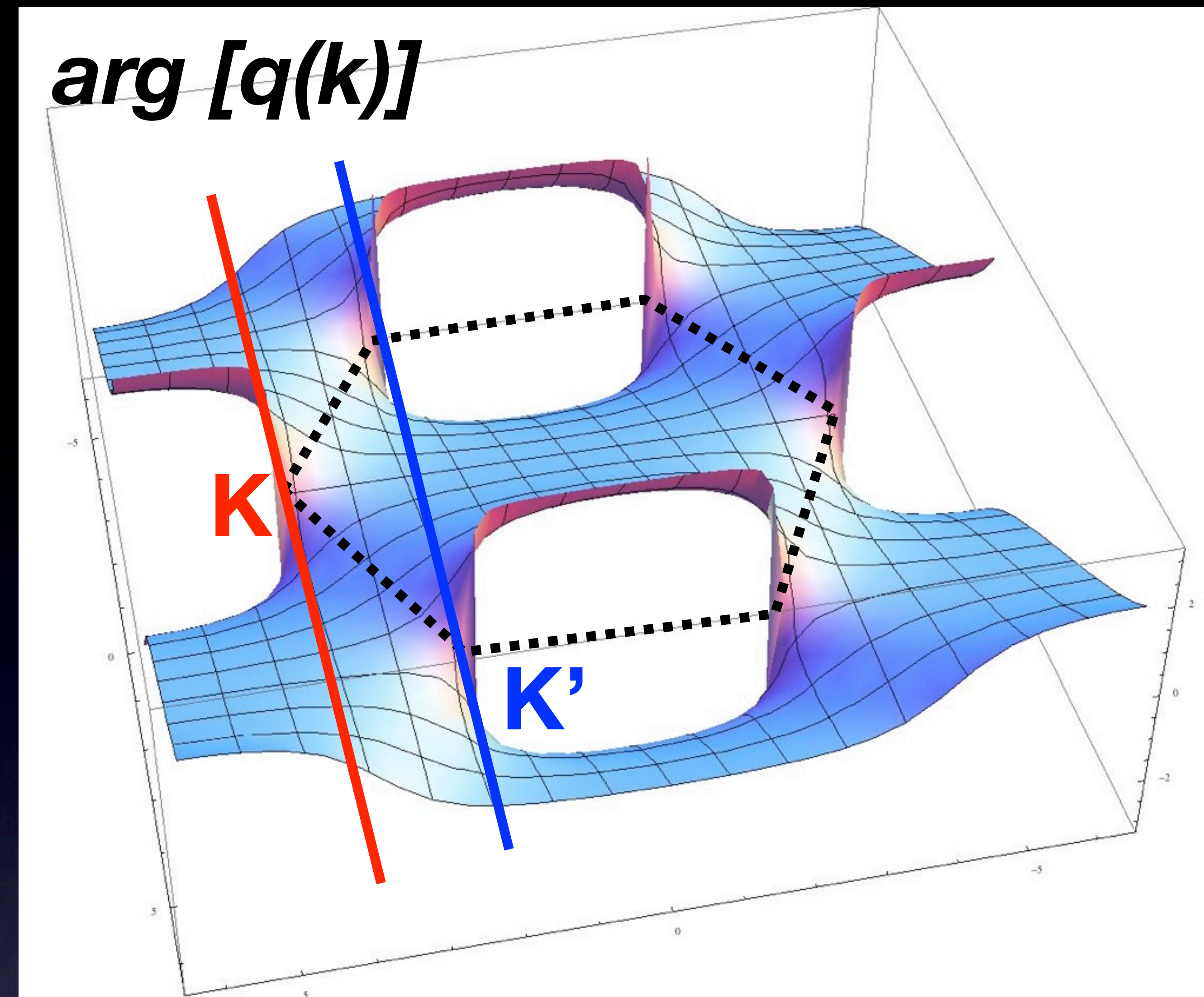
A winding number:

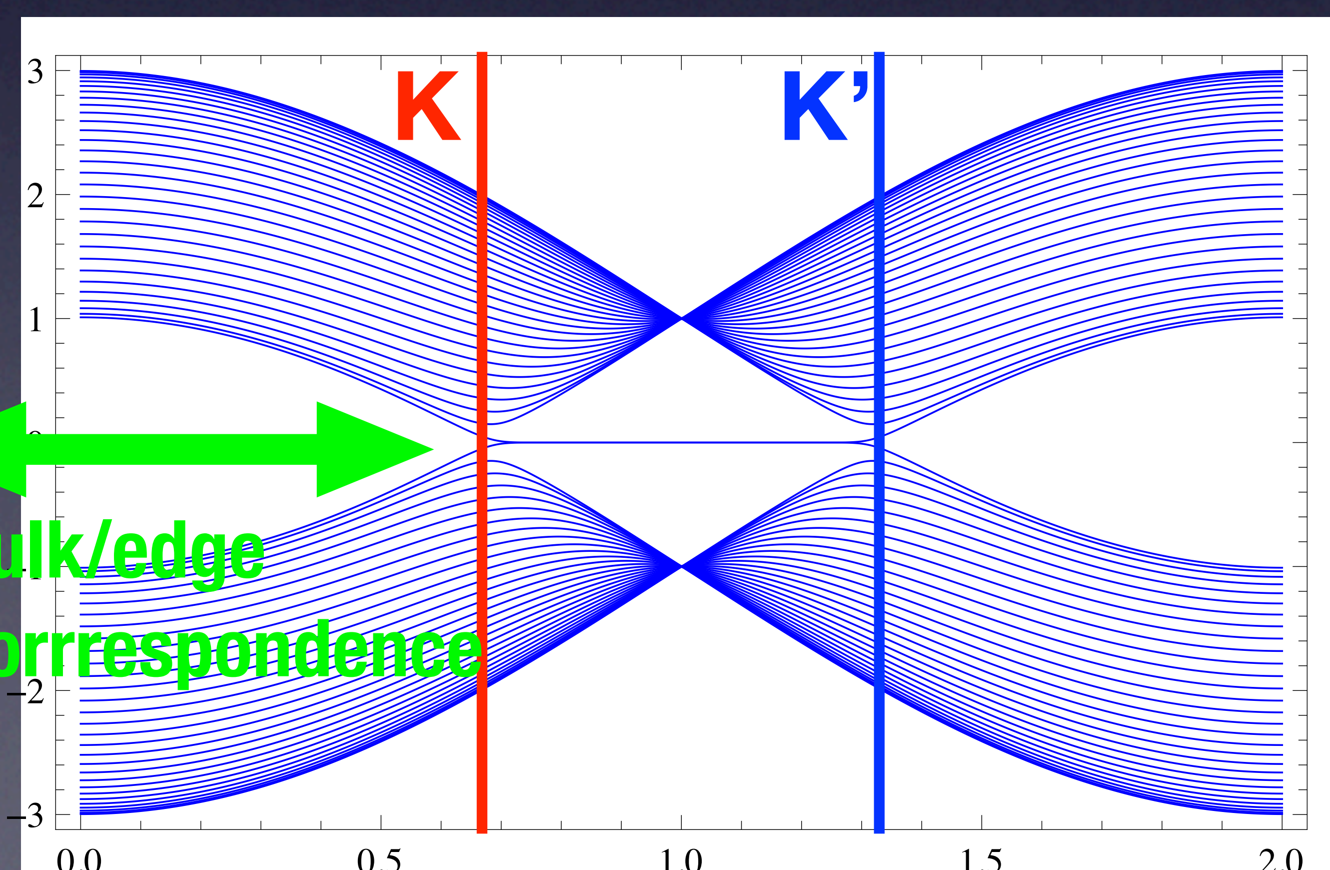
$$N_{\mathcal{L}} = \oint_{\mathcal{L}} \frac{dk}{2\pi} \, \mathrm{Tr}\, [q(\boldsymbol{k})^{-1} \partial_{k_{\mathcal{L}}} \, q(\boldsymbol{k})]$$

$$q(\boldsymbol{k}) = f(\boldsymbol{k})/|f(\boldsymbol{k})|$$

can be defined, protecting the existence of a pair of Dirac points: K & K'

Fujita, Wakabayashi, et al., JPSJ 65, 1920 (1996)



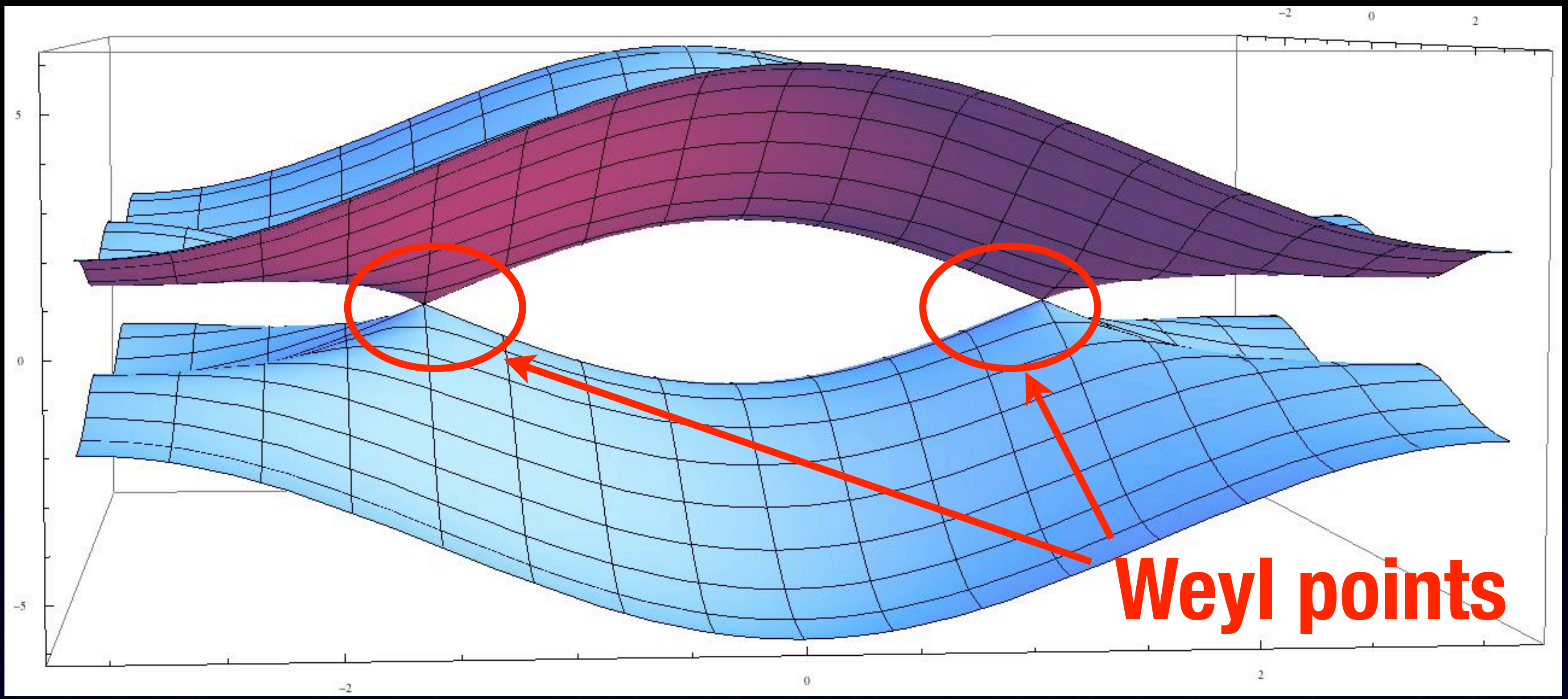


bulk/edge correspondence

Generalization to 3D

- Weyl semimetal
- class A
- protected point

node : Z-type



$$H = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$$
$$= A(k_x \sigma_x + k_y \sigma_y) + M(\boldsymbol{k}) \sigma_z$$

K.-Y. Yang et al. arXiv:1105.2353

$$M(\boldsymbol{k}) = \Delta(k_z) + B(k_x^2 + k_y^2) \qquad \Delta(k_z) = 2t_z(\cos k_z - \cos k_0)$$

A 2D Chern number number:

$$\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k}) / |\boldsymbol{d}(\boldsymbol{k})|$$

$$N_{S^2} = \int_{S^2} \frac{d\boldsymbol{k}}{8\pi} \epsilon_{\mu\nu} \, \boldsymbol{n}(\boldsymbol{k}) \cdot [\partial_{k_\mu} \boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_\nu} n(\boldsymbol{k})]$$

can be defined,
protecting the existence
of a pair of Weyl points at
kz = +k0, -k0 (kx = ky =0)

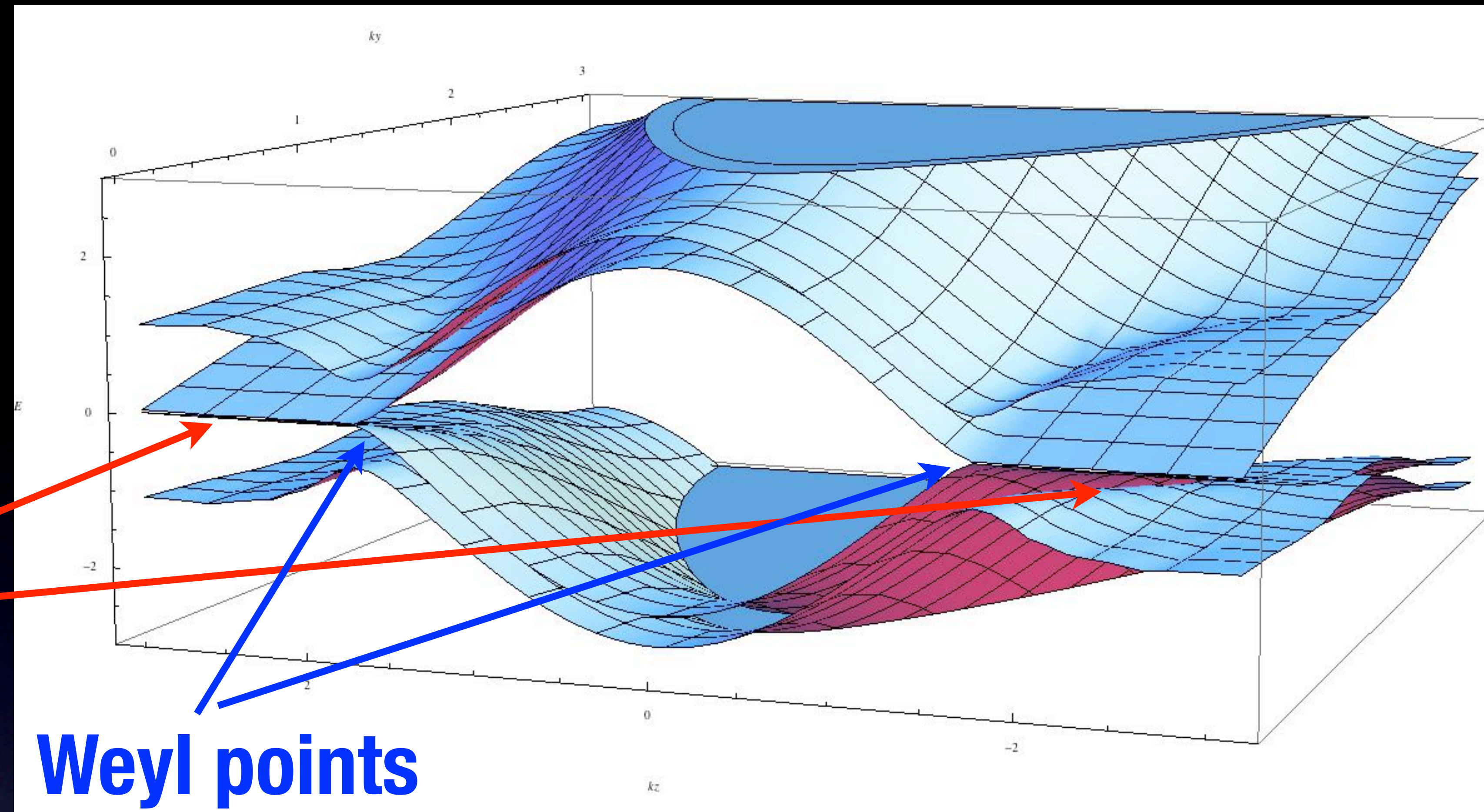
↔ **bulk/edge corrrespondence**

Fermi arc surface states

Protected surface states = Fermi arcs

geometry: a ***slab*** (0<x<L)

Fermi-arc surface states

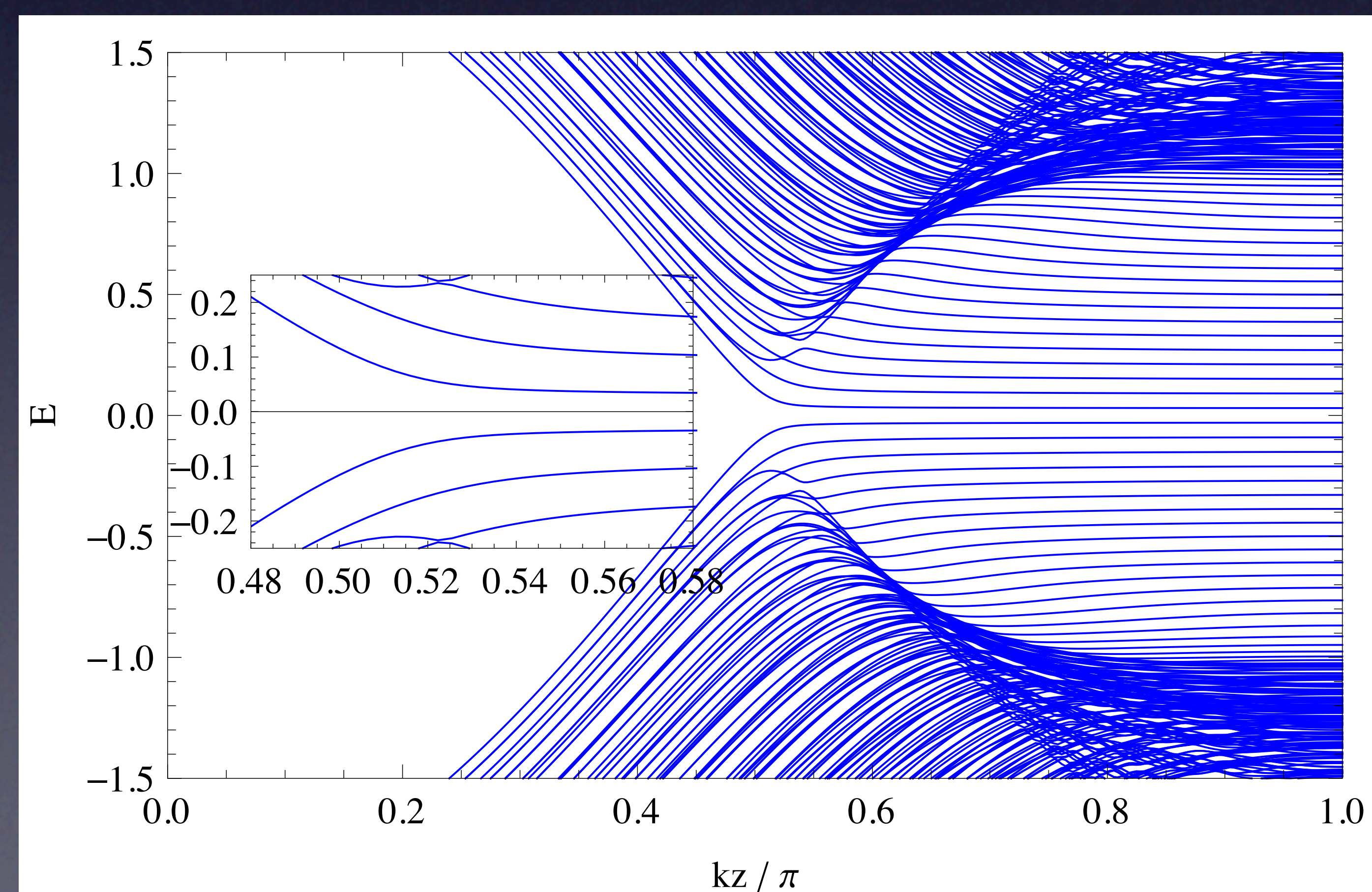


On a <u>cylinder</u>,

the Fermi-arc surface states split into <u>multiple completely flat subbands</u>

flatness: topologically protected

How about spin-to-surface locking?



Chiral spin-to-surface locking in the Fermi-arc surface states

Analytic calculation: • *repeating the same type of analysis...*

$$H = H_\perp + H_\parallel \qquad H_\perp(k_r) = H\big|_{k_\phi=0,k_z=k_z^{(0)}} \qquad |\psi(r=R,\phi,z)\rangle = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

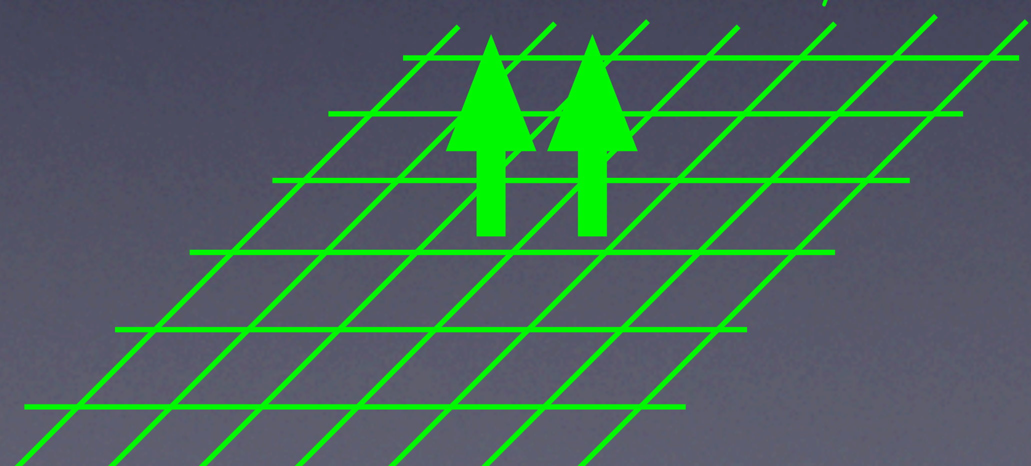
The basis eigenspinor: $$|\psi_\perp\rangle = \rho(r)\left(e^{\kappa_+(r-R)} - e^{\kappa_-(r-R)}\right)\begin{bmatrix} 1 \\ -ie^{i\phi} \end{bmatrix}$$

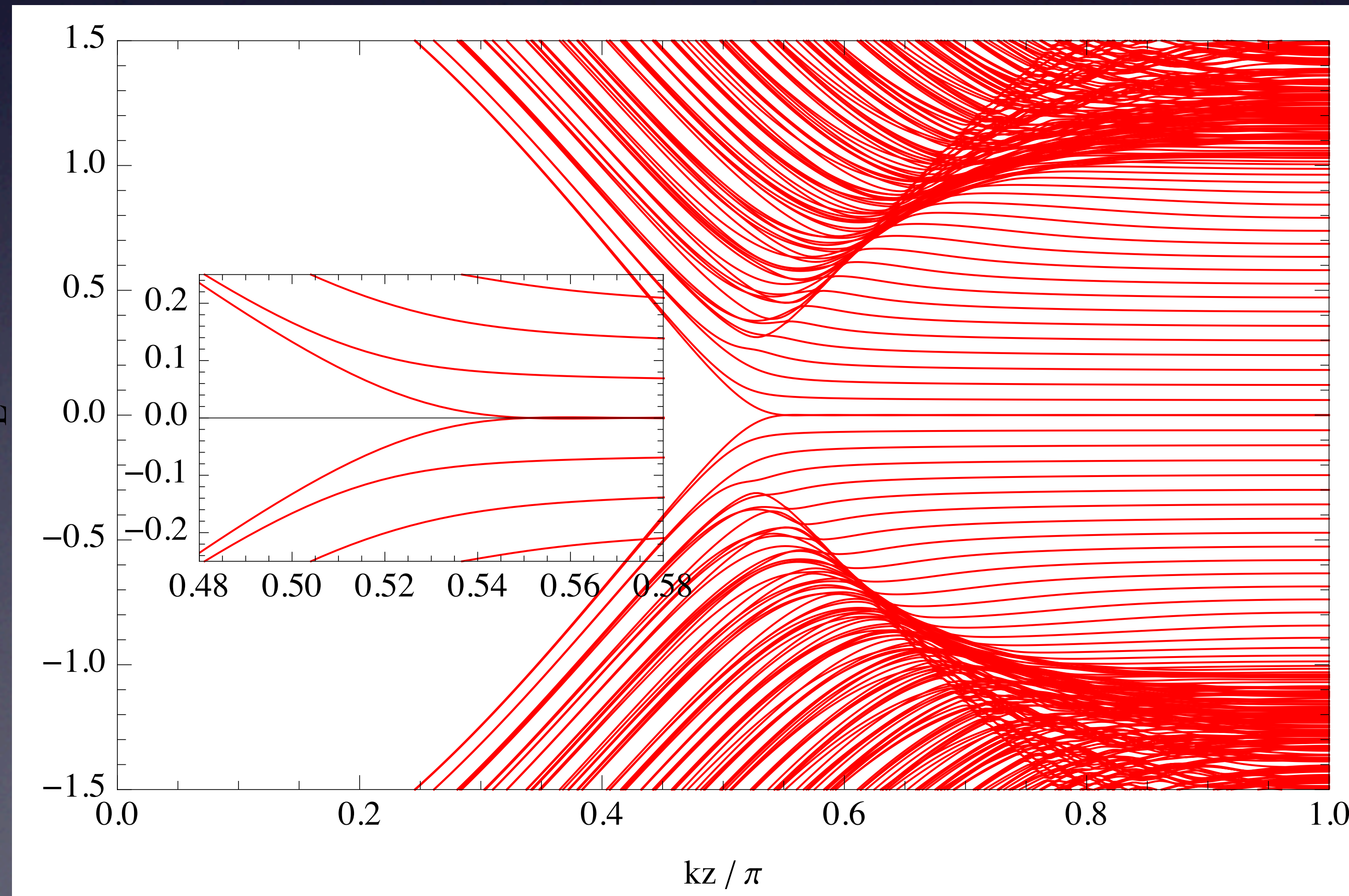
The surface effective Hamiltonian: $$H_{\text{surf}} = \langle\psi_\perp|H_\parallel|\psi_\perp\rangle = \frac{A}{R}\left(-i\frac{\partial}{\partial\phi} + \frac{1}{2}\right)$$

Numerics:

• *confirmed the closing of the gap in the presence of*

$$\Phi_{AB} = \pi/2 \times 2$$





Conclusions

Gapped case : weak & strong topological insulators

- ***half-integer*** quantization of the ***orbital*** angular momentum
- ***algebraic*** (extremely slow of) decay of ΔE
- gapless helical modes along dislocation lines: role of ***weak*** indices:

"How weak is a weak topological insulator?"

C.-X. Liu, KITP 2011; R. Mong, Station Q, tomorrow

Ringel, Kraus, Stern, arXiv:1105.4351

Gapless case : Weyl semimetal / Fermi arc surface states

- completely ***flat*** multiple subbands
- flatness: topologically protected!
- ***chiral*** spin-to-surface locking: spin locked to the ***azimuthal*** component of the momentum

Acknowledgments: A. Schnyder, M. Sato, A. Ludwig, C.L. Kane, Y.-B. Kim, E.-G. Moon, A. Yamakage, T. Fukui, Y. Tanaka, ..., many other people

supplementary slides

Relation to
the periodic table, "the ten-fold way"

A. Schnyder et al., PRB '09; NJP '10; A. Kitaev, AIP '10

Classification in the presence of toplogical defects:

Teo & Kane, PRB 82, 115120 (2010)

"The weak indices are related to the strong indices in one lower dimension."

Ran, arXiv:1006.5454; A. Schnyder et al. NJP '10

"(d-1) indices"

"It is these (d-1) indices that control the existence of one-dimensional helical modes hosted by dislocations."

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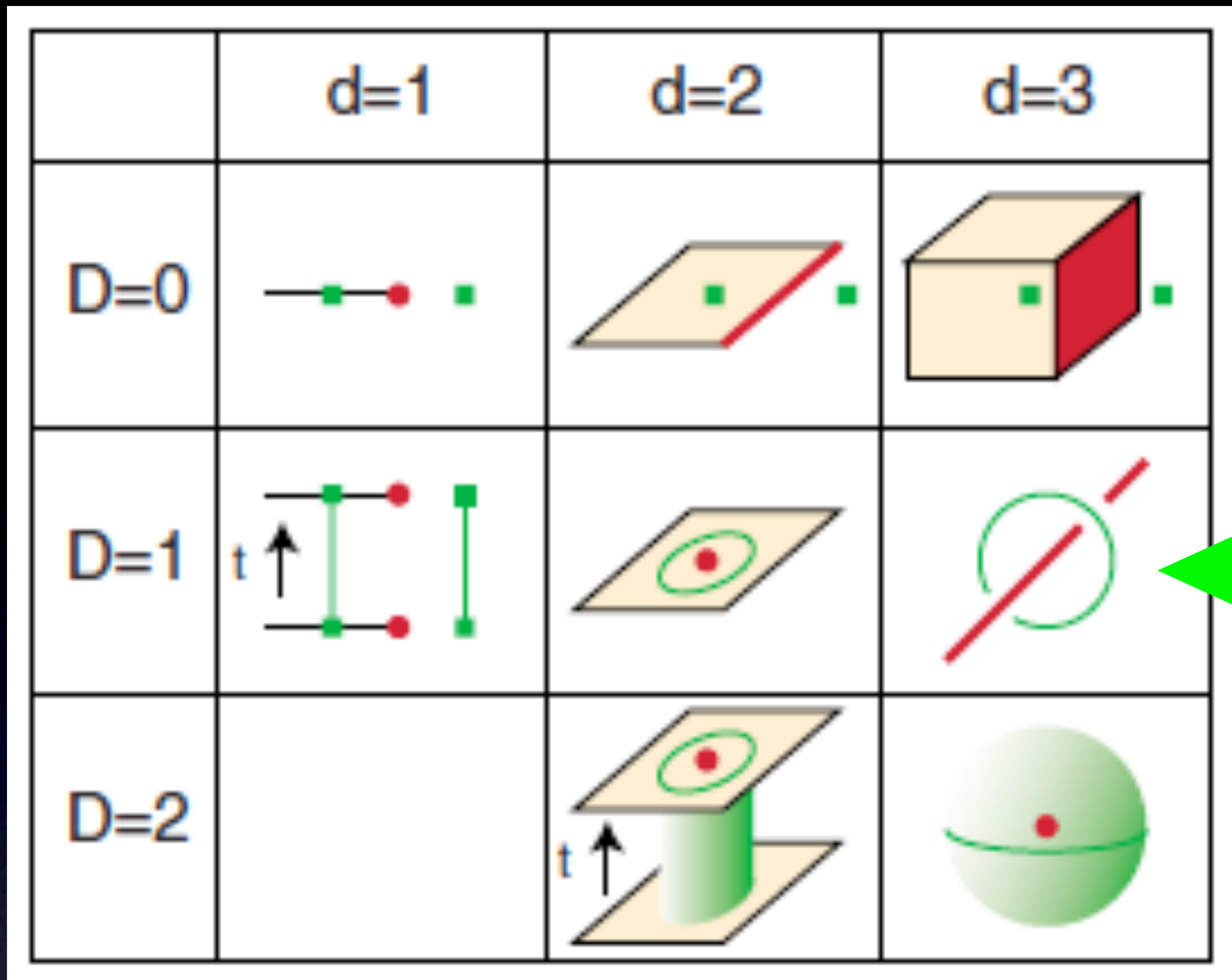
	strong	*weak*	
d=3	ν_0	(ν_1, ν_2, ν_3)	*2D gapless surface Dirac cone*
d-1=2	ν_3		*1D gapless helical modes*



The periodic table: *Teo-Kane's version*

Teo & Kane, PRB 82, 115120 (2010)

d=3
D=1   d-D=d-1=2

- the ***effective*** spatial dimension:

$$d \rightarrow \delta = d - D$$

symmetry class

	T	C	Γ_5	0	1	2	3	4	5	6	7
A	0	0	0	Z	0	Z	0	Z	0	Z	0
AIII	0	0	1	0	Z	0	Z	0	Z	0	Z
AI	1	0	0	Z	0	0	0	Z	0	Z_2	Z_2
BDI	1	1	1	Z_2	Z	0	0	0	Z	0	Z_2
D	0	1	0	Z_2	Z_2	Z	0	0	0	Z	0
DIII	-1	1	1	0	Z_2	Z_2	Z	0	0	0	Z
AII	-1	0	0	Z	0	Z_2	Z_2	Z	0	0	0
CII	-1	-1	1	0	Z	0	Z_2	Z_2	Z	0	0
C	0	-1	0	0	0	Z	0	Z_2	Z_2	Z	0
CI	1	-1	1	0	0	0	Z	0	Z_2	Z_2	Z