Emergent topological phenomena in antiferromagnets with noncoplanar spins

- Surface quantum Hall effect
- Dimensional crossover

Bohm-Jung Yang

(RIKEN, Center for Emergent Matter Science (CEMS), Japan)

Collaborators

- Naoto Nagaosa (U. Tokyo and RIKEN)
- Mohammad Saeed Bahramy (RIKEN)

Outline

0. Introduction

- Quantum Hall effect without magnetic field
- Topological phenomena in noncoplanar magnets

1. Surface quantum Hall effect

- Noncoplanar spin ordering in pyrochlore antiferromagnet
- Topologically protected bound state in a continuum

2. Dimensional crossover in thin films of pyrochlore iridates

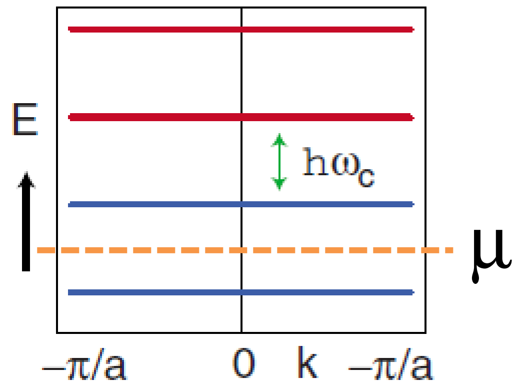
- Giant anomalous Hall effect
- New topological phase: anti-Chern insulator

Quantum Hall effect under magnetic field

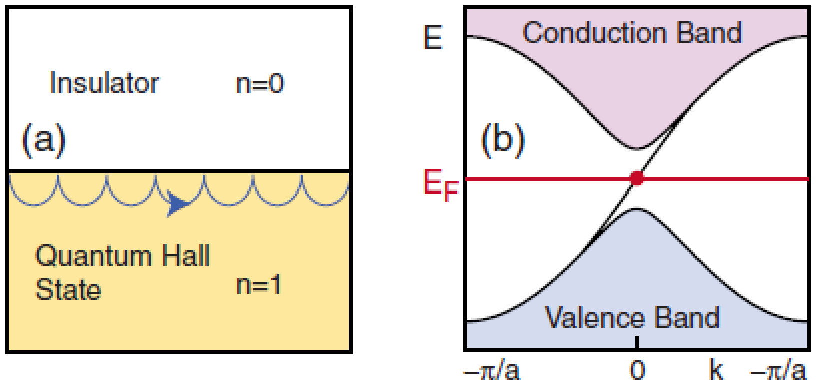
- Quantized Hall conductivity

$$\boxed{\sigma_{xy} = C\frac{e^2}{h},}$$

$C = 0, 1, 2, \ldots.$



- Boundary gapless modes



- Berry phase induced topological response

TKNN invariant :

$$C = \frac{1}{2\pi}\int d^2k F, \qquad F = \nabla \times A, \qquad A = i\langle u(\mathbf{k})|\nabla_k|u(\mathbf{k})\rangle,$$

Thouless, Kohmoto, Nighingale, Nijs (1982)

Quantum Hall effect without magnetic field

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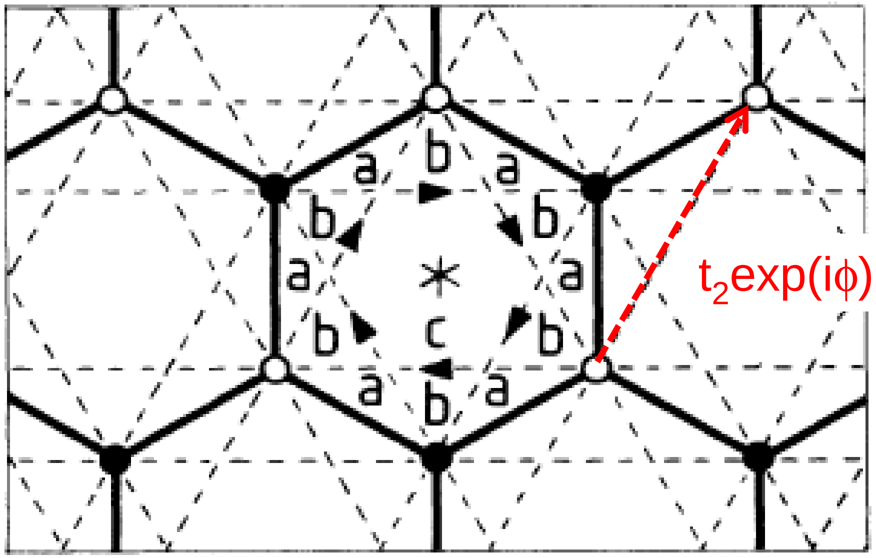
Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)



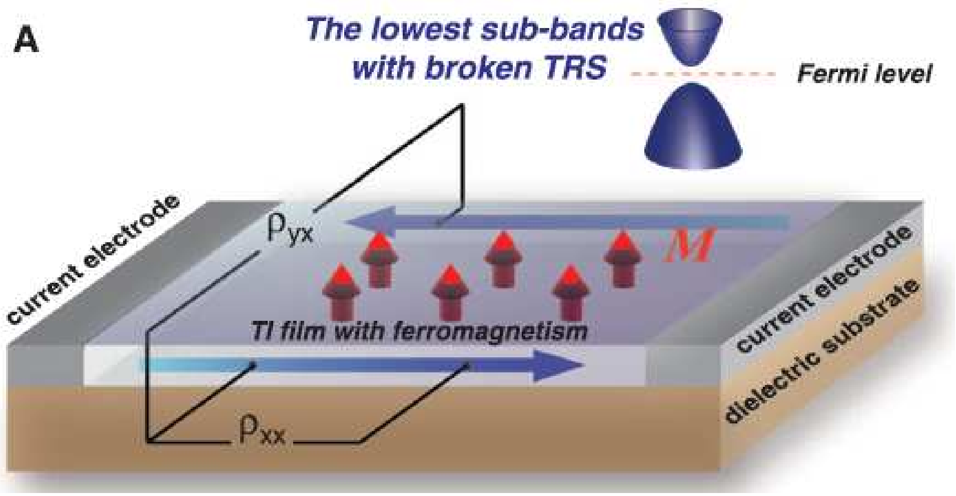
Current loop (imaginary hopping) can generate quantum Hall insulator!

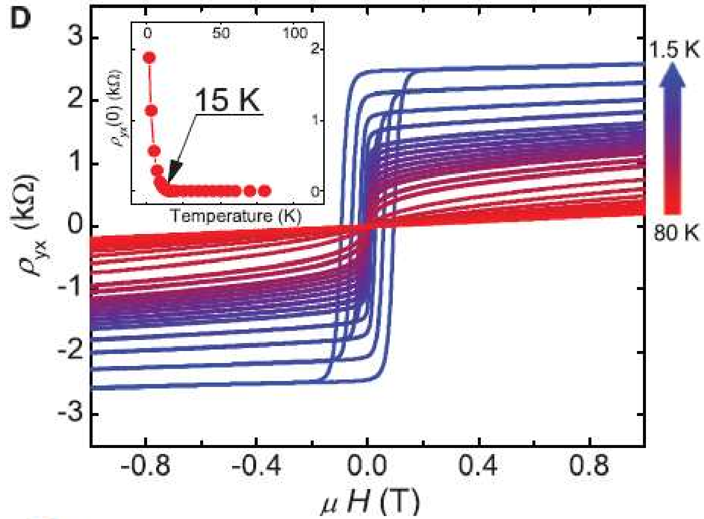
Quantum anomalous Hall effect in TI

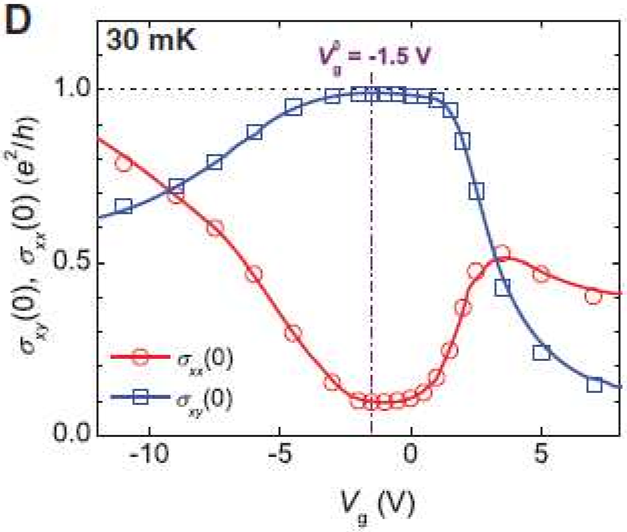
- On the surface of 3D topological insulator with bulk ferromagnetism

$Cr_{0.15}(Bi_{0.1}Sb_{0.9})_{1.85}Te_3$

C.-Z. Chang, Q.-K. Xue, Science (2013)



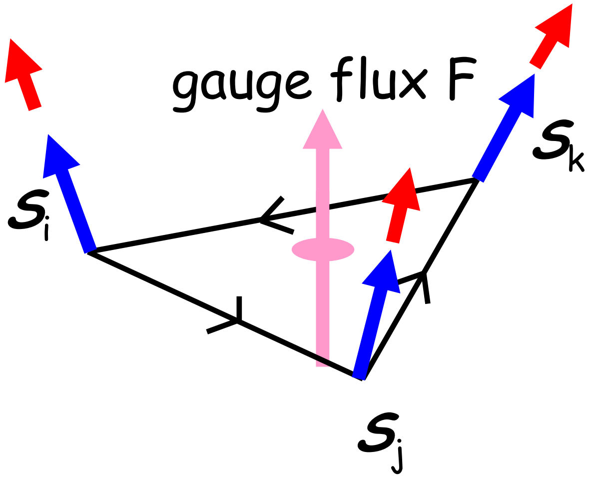




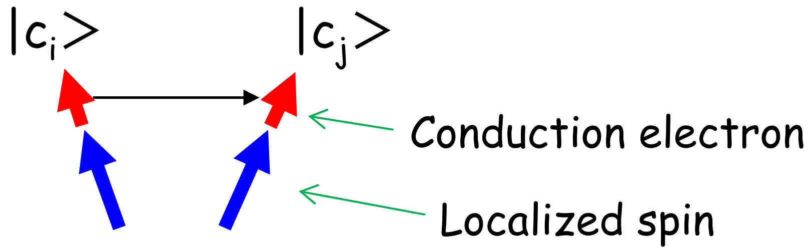
2D massless Dirac particle on surface

$$H = \hbar v_{\mathrm{F}}(\mathbf{k}\times\hat{\mathbf{z}})\cdot\boldsymbol{\sigma} - J n_s \bar{S}_z \sigma_z$$

Berry phase due to non-coplanar spin



$$\text{Loop} : i \to j \to k \to i$$



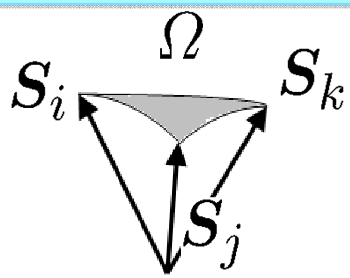
$$t_{ij}^{\text{eff}} = t_{ij}\langle \chi_i | \chi_j \rangle = t_{ij} e^{i a_{ij}} \cos\left(\frac{\theta_{ij}}{2}\right)$$

acquire a phase factor = Berry phase

Fictitious flux (in a continuum limit)

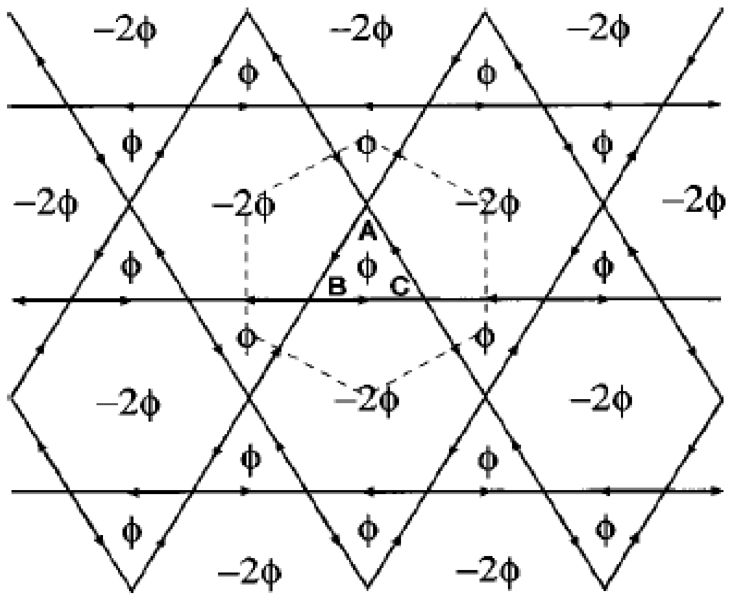
$$\Phi \propto \frac{\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)}{2} = \frac{\Omega}{2}$$

scalar spin chirality



Quantum Hall effect in non-coplanar magnets

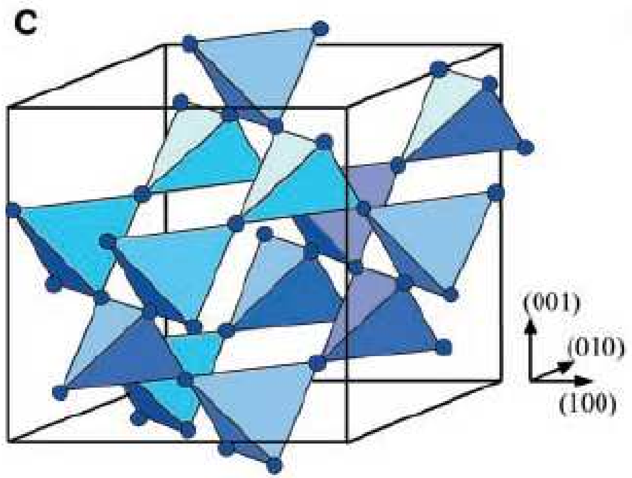
$$H=\sum_{NN} t_{ij}\psi^{\dagger}_{i\sigma}\psi_{j\sigma}-J_H\sum_{i} \psi^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_i\psi_{i\beta}\,,$$



Ohgushi, Murakami, Nagaosa

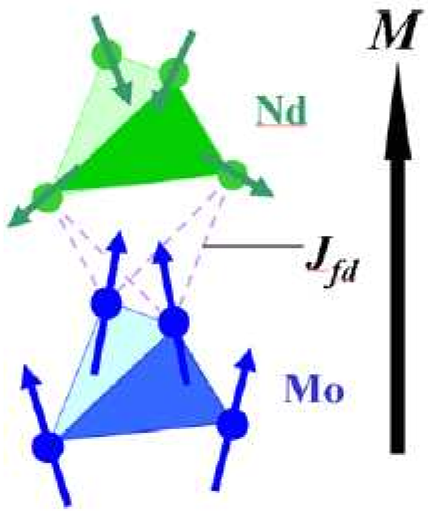
Spin Berry phase can generate quantum Hall effects

Anomalous Hall effect in pyrochlore magnets

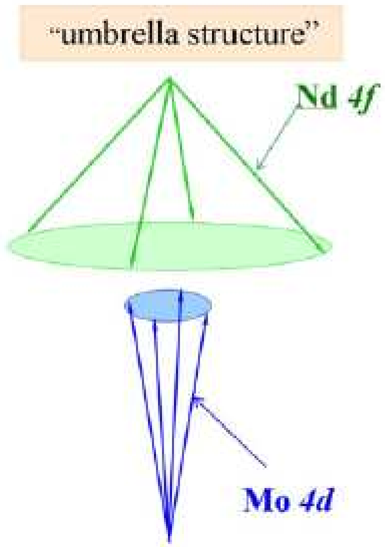


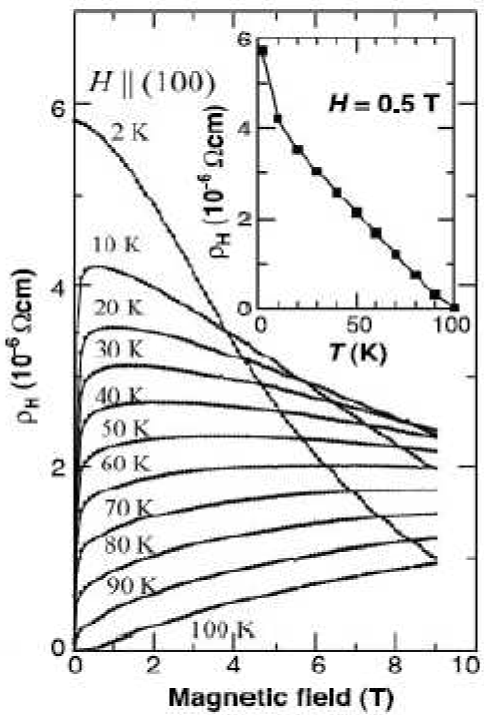
$Nd_2Mo_2O_7$

Localized



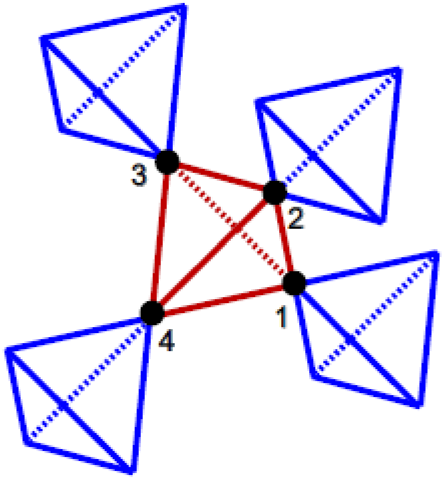
Itinerant





Taguchi, Nagaosa, Tokura (2001)

Spin Berry phase in pyrochlore lattice

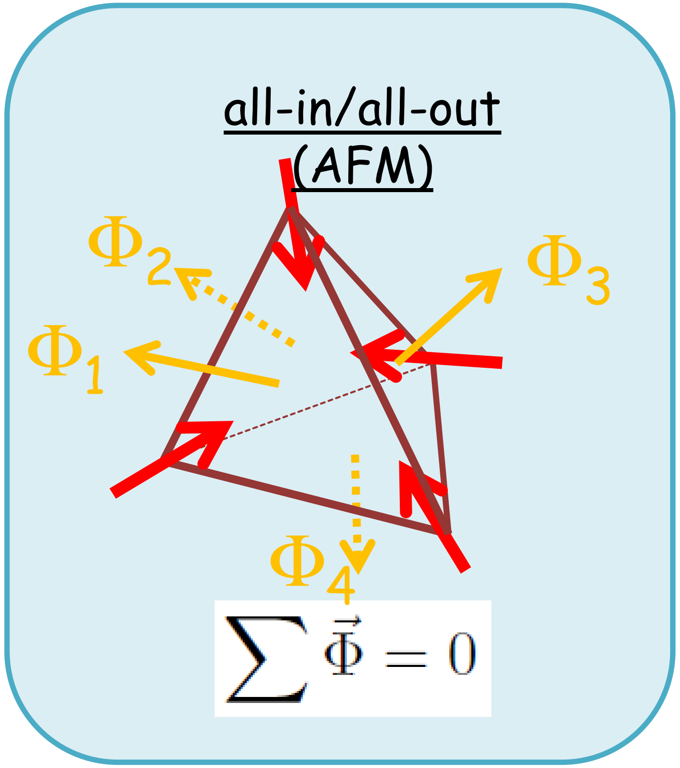


Noncoplanar magnetic ordering (spin anisotropy)

- $R_2Mo_2O_7$ (R=Nd, Sm, Gd): 2-in/2-out
- $Cd_2Os_2O_7$, $A_2Ir_2O_7$ (A=Nd, Sm, Eu) : all-in/all-out

Systems with broken lattice symmetry
: Surface, film, distortion …

New emergent topological phenomena

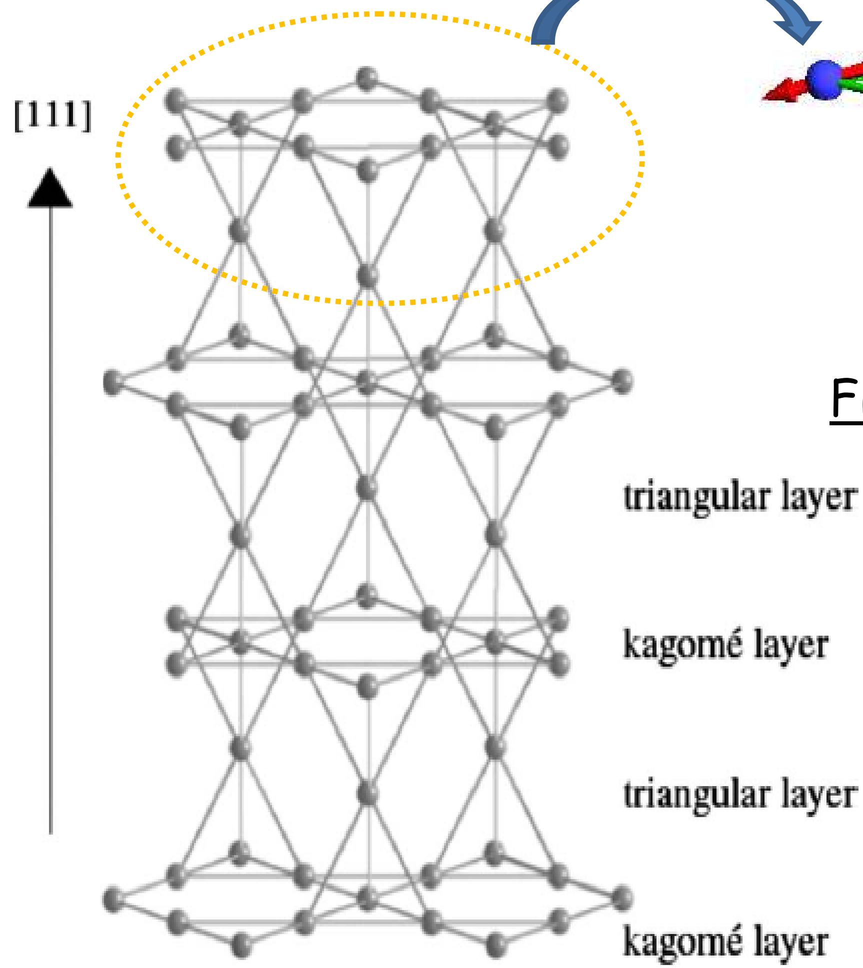


1. Surface quantum Hall states

- Spin Berry phase in antiferromagnets with non-coplanar spins
- Topologically protected bound state in a continuum

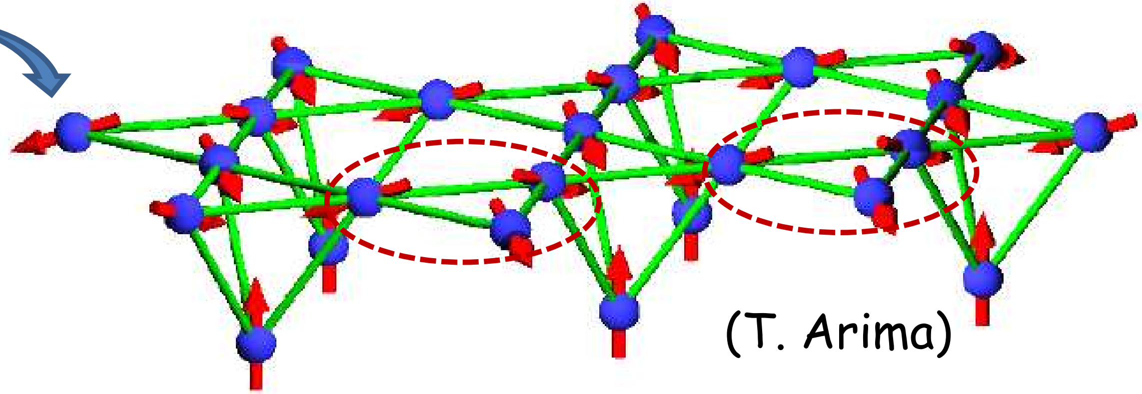
- **<u>B. -J. Yang</u>**, M. S. Bahramy, and N. Nagaosa, Nature Communications 4, 1524 (2013).

Surface QHE in pyrochlore all-in/all-out AFM



Gardner et al. RMP (2010)

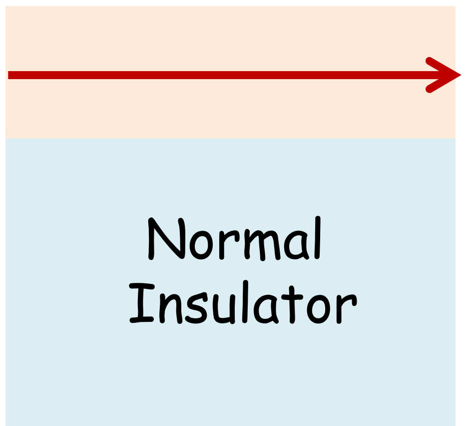
Kagome layer on the surface



(T. Arima)

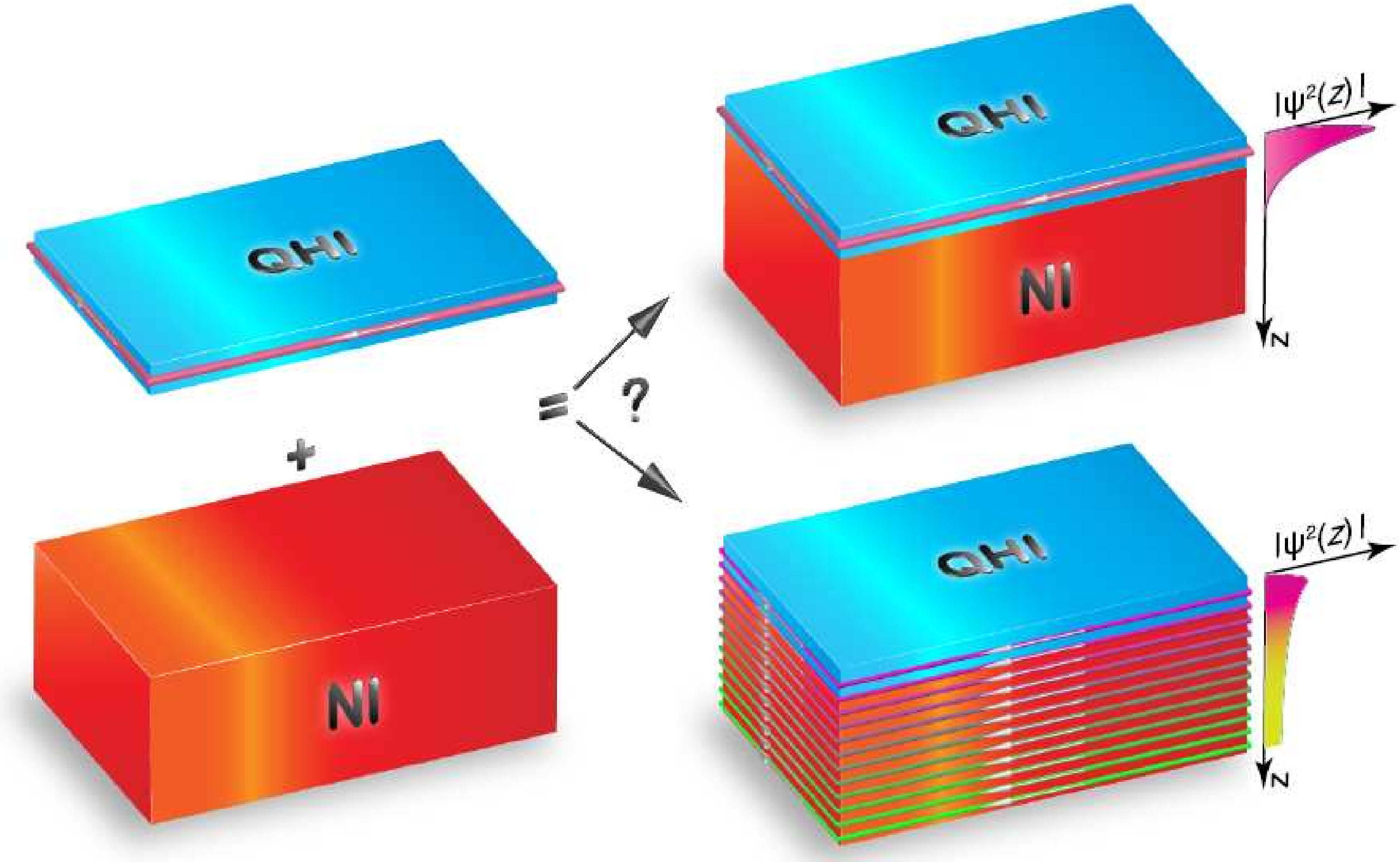
Finite effective magnetic field on the surface!

Surface QH



Is it
stable ?

Stability of surface quantum Hall states

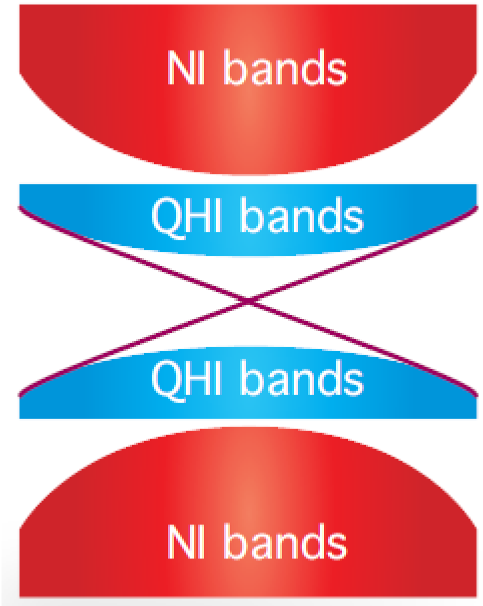


Localization of wave functions of QHI ? Chern number dilution ?

Band structure of the heterostructure

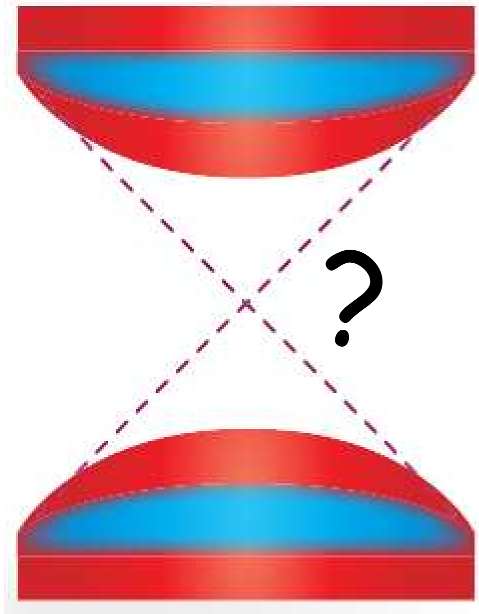
- Energy dispersion E(k)

(1) Decoupled bands



1D edge and 2D bulk states of QHI can be localized on the top layer

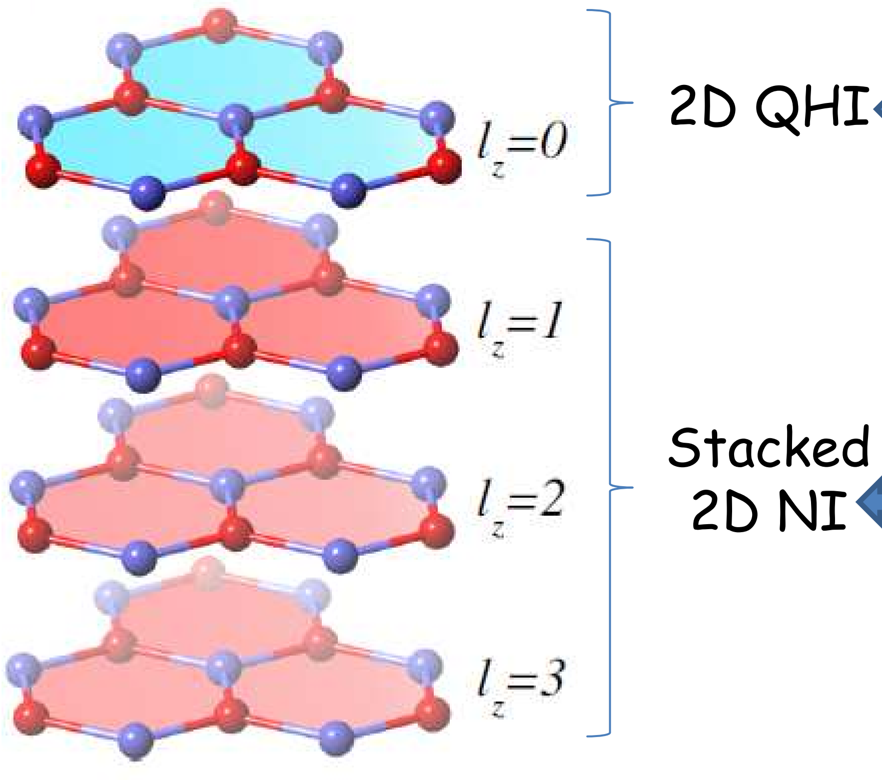
(2) Fully coupled bands

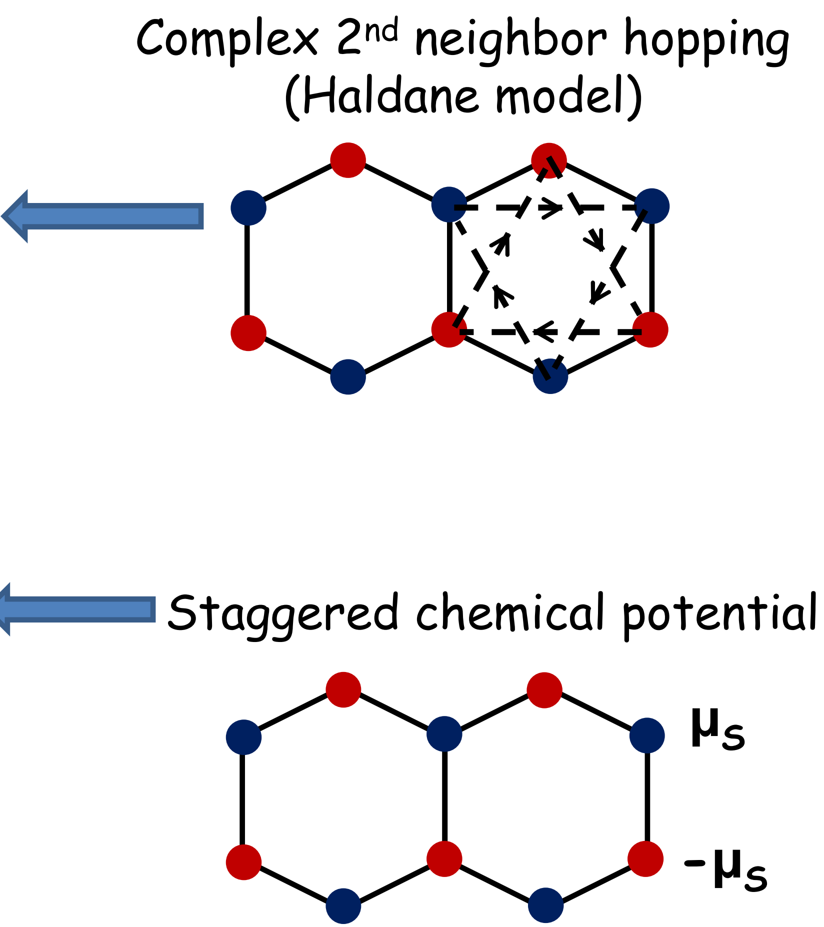


Spatial distribution of 1D edge and 2D bulk states of QHI ?

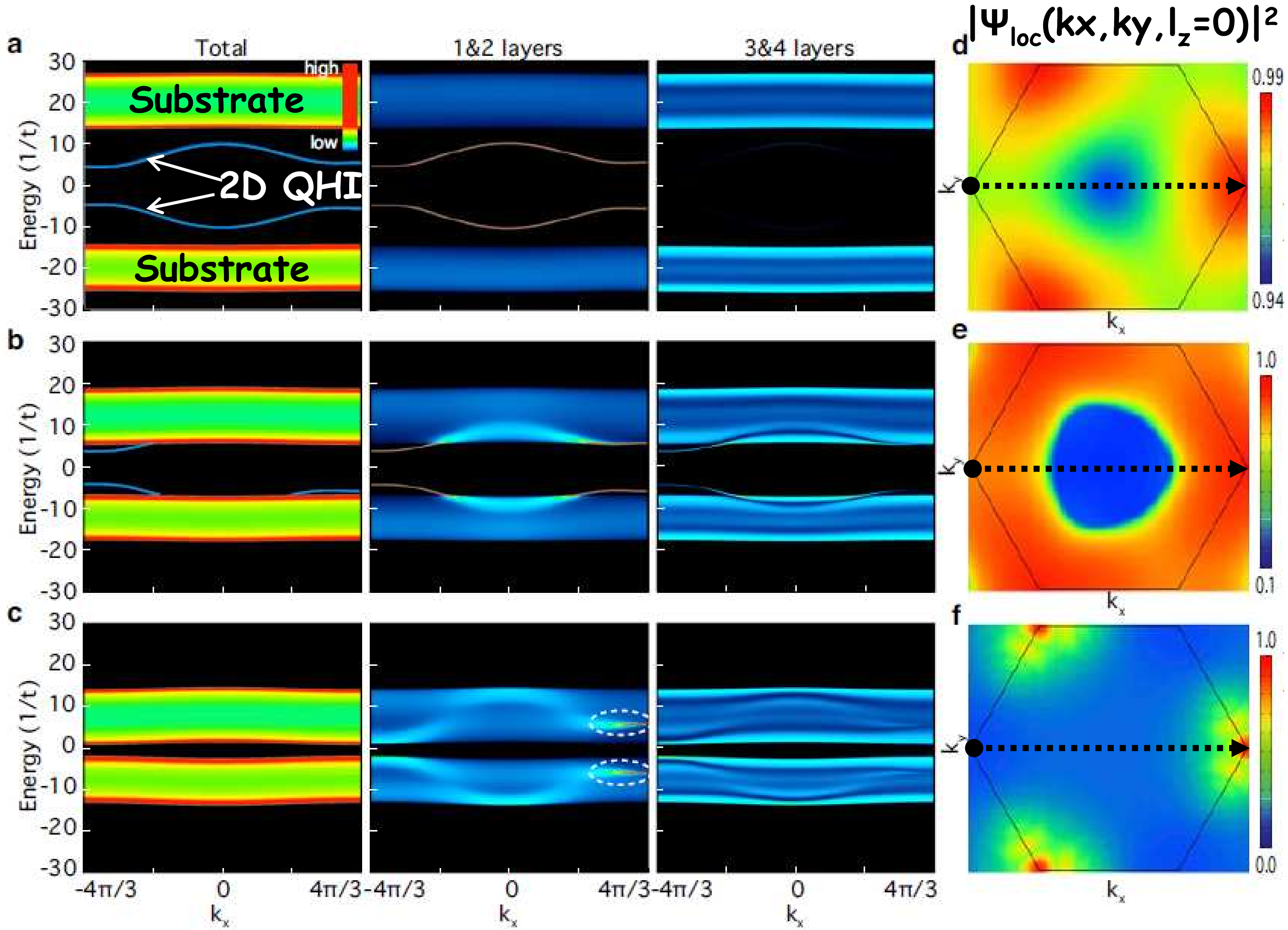
Stacked honeycomb lattice model

Simplest model with two-bands

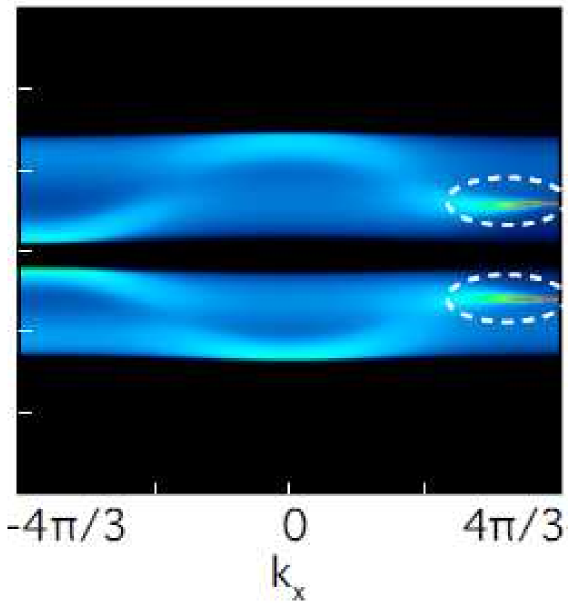


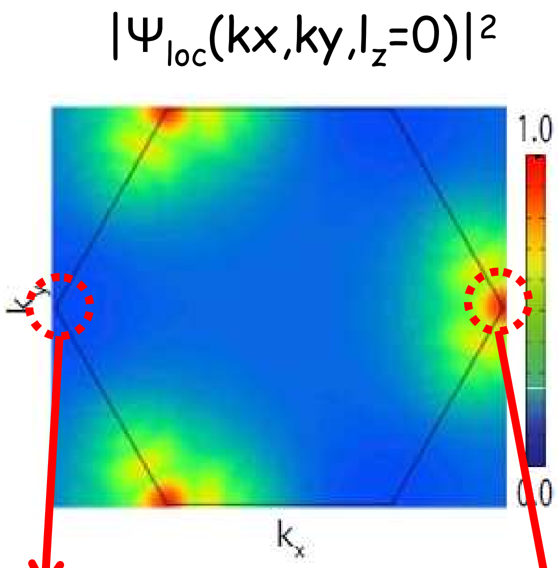


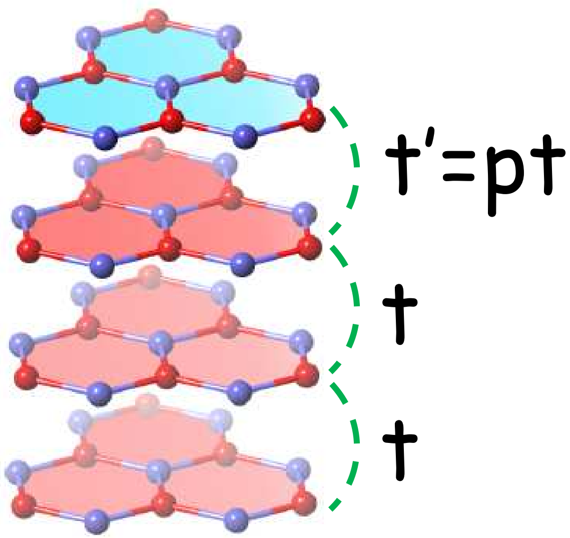
Layer-resolved wave function distribution

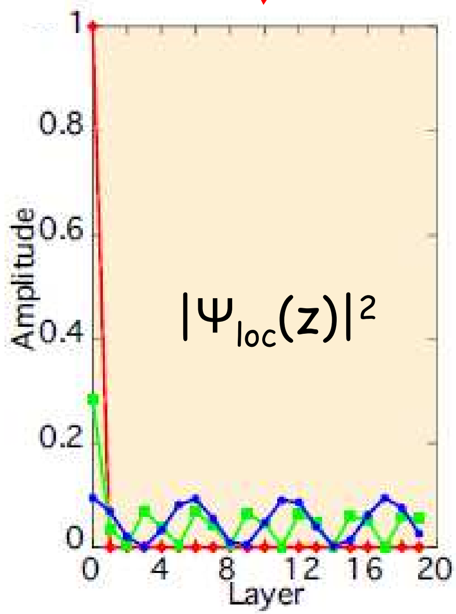


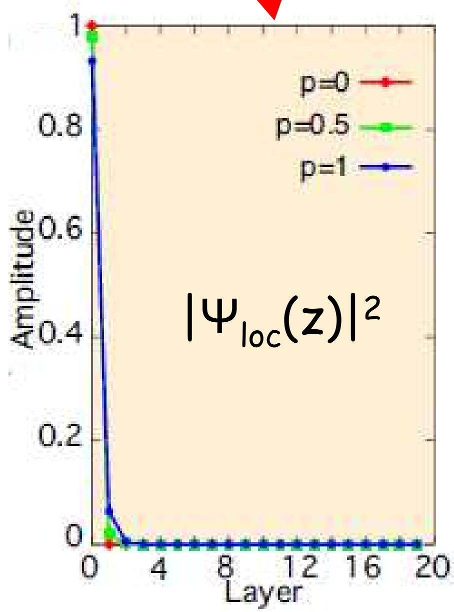
Localized bound state in a continuum





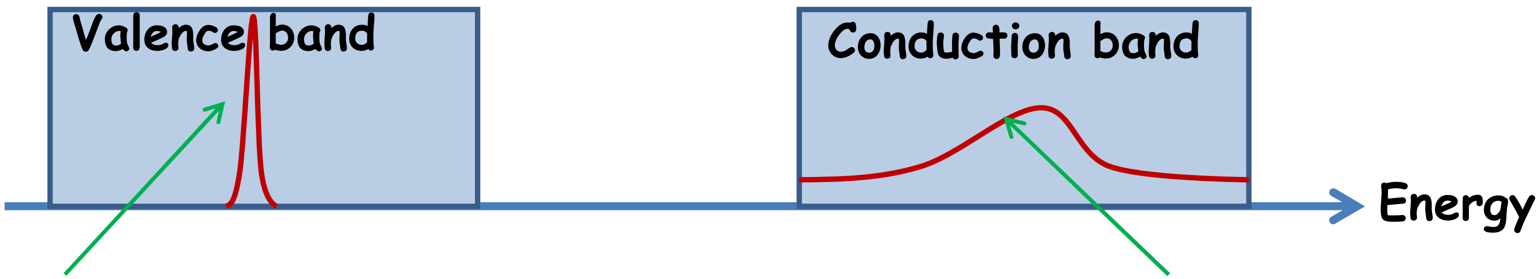






Description of the localized bound state

- Use Green's function of quantum Hall insulator



Localized state (a pole of G^R)

$$\mathrm{Im}[G^R(\omega)]^{-1} = -\pi\delta(\omega - \epsilon_0 - \mathrm{Re}\Sigma),$$

Extended state

$$\mathrm{Im}[G^R(\omega)]^{-1} = -\frac{\mathrm{Im}\Sigma}{(\omega-\epsilon_0-\mathrm{Re}\Sigma)^2+\mathrm{Im}\Sigma^2},$$

- Two-band Fano model : $H = H_{\mathrm{QHI}} + H_{\mathrm{substrate}} + H_{\mathrm{hybridization}},$

$$\boxed{H_{\mathrm{QHI}}(\vec{k}_\perp) = \vec{h}\cdot\vec{\tau}} \qquad \boxed{H_{\mathrm{substrate}}(\vec{k}_\perp, k_z) = H_0 + \vec{H}\cdot\vec{\tau},}$$

Integrate out substrate

$$\boxed{G_R^{-1}(\Omega) = \Omega - \vec{h}\cdot\vec{\tau} + i\frac{\Gamma}{2}\Big[1 + a_x\tau_x + a_y\tau_y + a_z\tau_z\Big],}$$

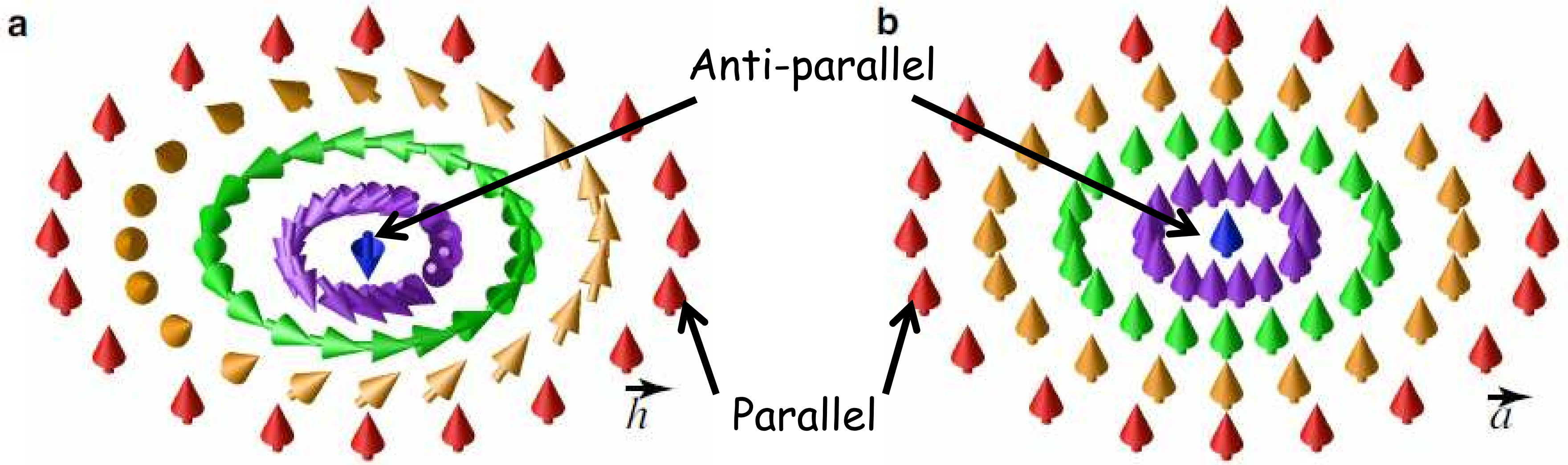
Topological protection of the bound state

$$H_{\mathrm{QHI}} = \vec{h} \cdot \vec{\tau}$$
$$H_{\mathrm{substrate}} = H_0 + \vec{H} \cdot \vec{\tau}$$
$$\vec{a} = \pm \frac{\vec{H}}{|\vec{H}|}$$

- Bound state pole : $\boxed{\Omega = -\vec{a} \cdot \vec{h} = \pm|\vec{h}|.}$

(1) If $\vec{a} = \frac{\vec{h}}{|\vec{h}|}$, the pole appears at $\Omega = -|\vec{h}|$ ⟹ 3D bulk valence band

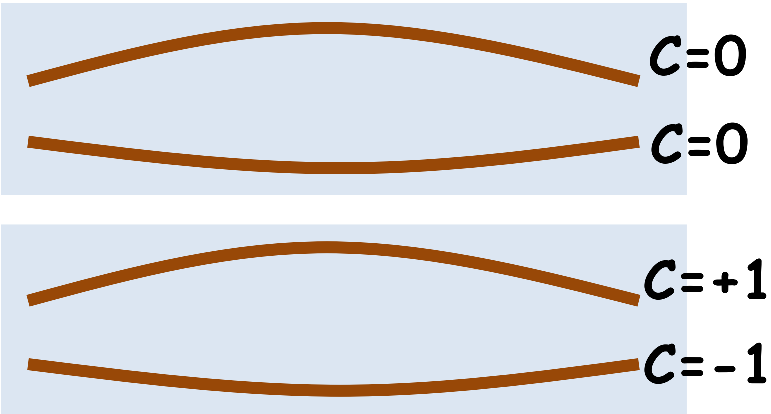
(2) If $\vec{a} = -\frac{\vec{h}}{|\vec{h}|}$, the pole appears at $\Omega = |\vec{h}|$ ⟹ 3D bulk conduction band

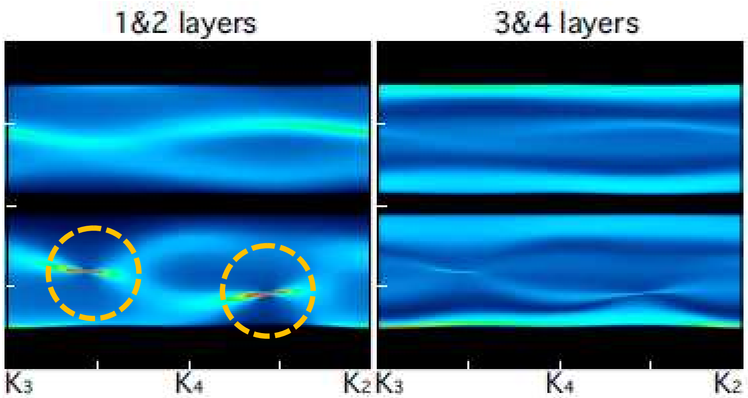


The localized bound state in the continuum is protected by the topology of h and a !

Generalization

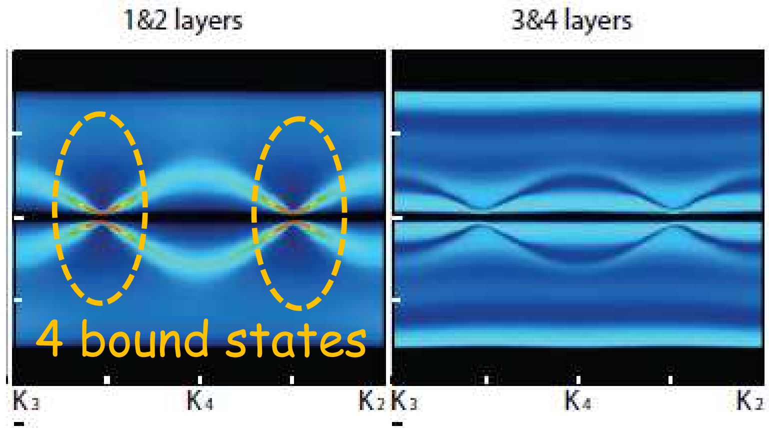
- **Multi-band systems**

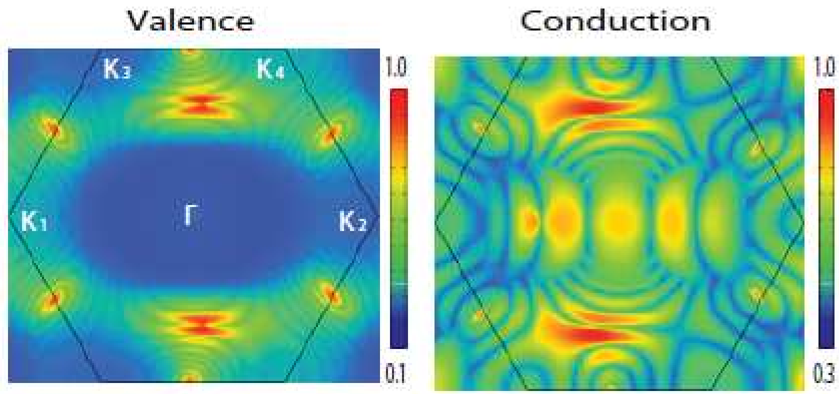




Only bands with finite Chern number support localized bound states !

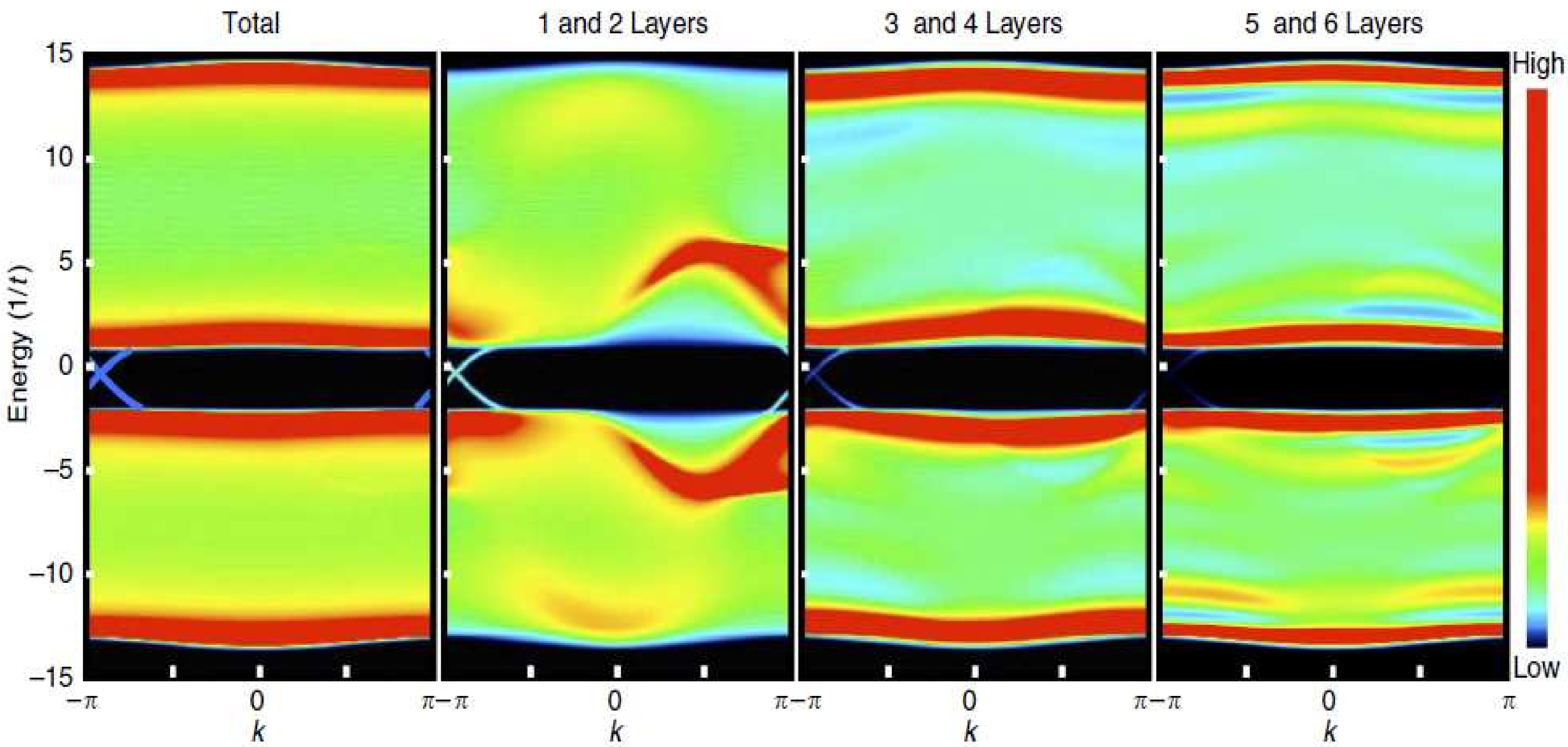
- **2D QHI with Chern number 2**





Chern number of the 2D band = minimum number of localized bound states!

Localization of edge states



Edge channel is exponentially localized along z-direction
as long as the energy is within the 3D bulk gap

Conclusion of part 1

1.Surface quantum Hall state is stable against hybridization.

2. The minimal number of localized bulk states is given by the Chern number difference between 2D QHI and the effective 2D NI system.

3. The 1D chiral edge state is localized as along as it appears within a bulk band gap.

1D chiral edge or some 2D bulk of QHI

Pyrochlore iridate does not show surface quantum Hall states.
But instead we have found an even more interesting state there!

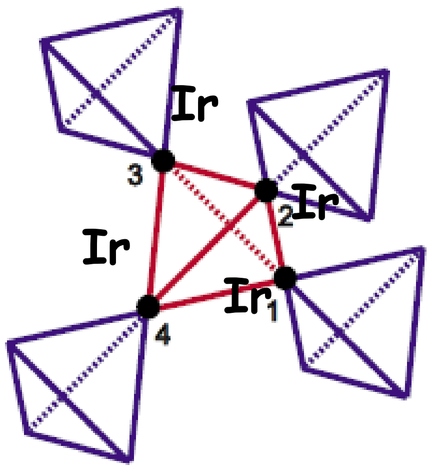
2. Dimensional crossover in pyrochlore iridate

- Emergent topological property in thin films of pyrochlore iridates

- **B. -J. Yang** and N. Nagaosa, submitted.

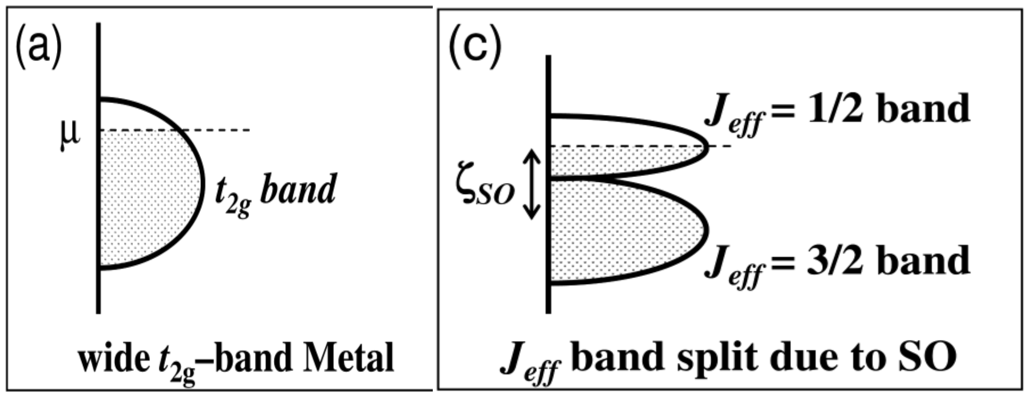
Pyrochlore iridates

$R_2Ir_2O_7$,R=Nd, Sm, Eu, Y



Ir^{4+} : 5 electrons in t_{2g}
with strong spin-orbit

1. Reduced bandwidth (B.J.Kim ,J.Yu, T.W.Noh et al.)



2. Berry phase effect due to J=1/2 states

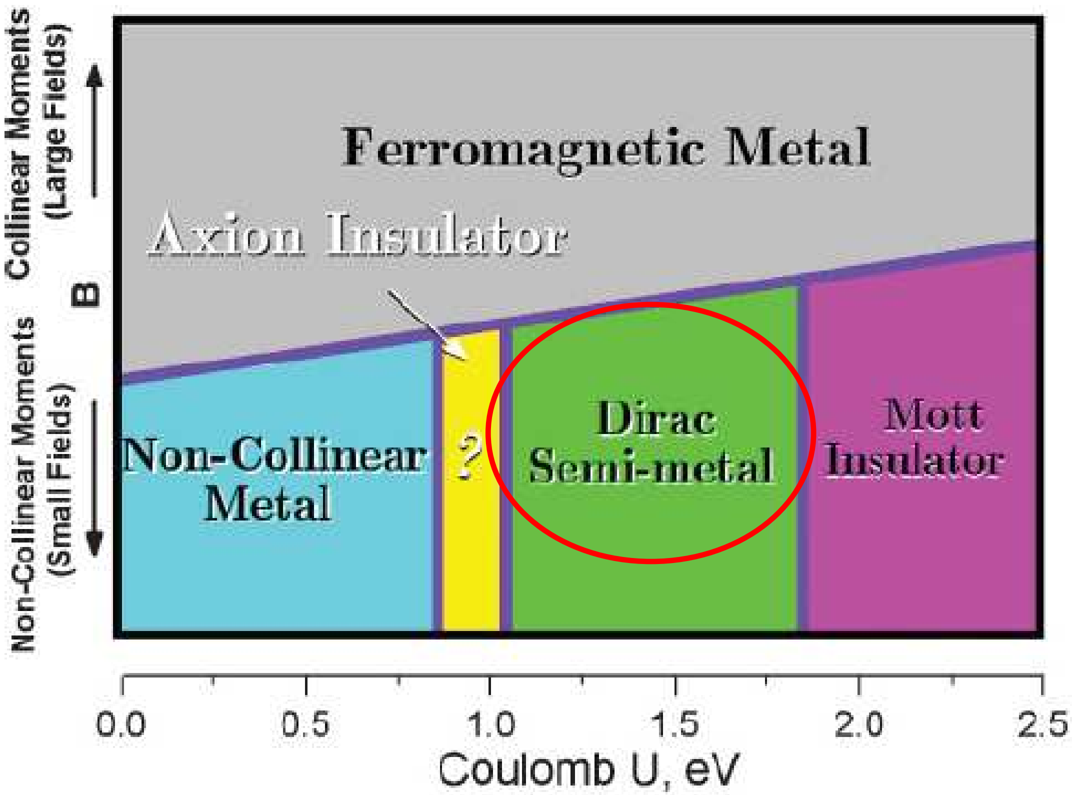
$$|j_z = +1/2\rangle = (+|xy\uparrow\rangle + |yz\downarrow\rangle + i|zx\downarrow\rangle)/\sqrt{3},$$
$$|j_z = -1/2\rangle = (-|xy\downarrow\rangle + |yz\uparrow\rangle - i|zx\uparrow\rangle)/\sqrt{3},$$

Spin-orbit coupling ≅ bandwidth ≅ Coulomb interaction

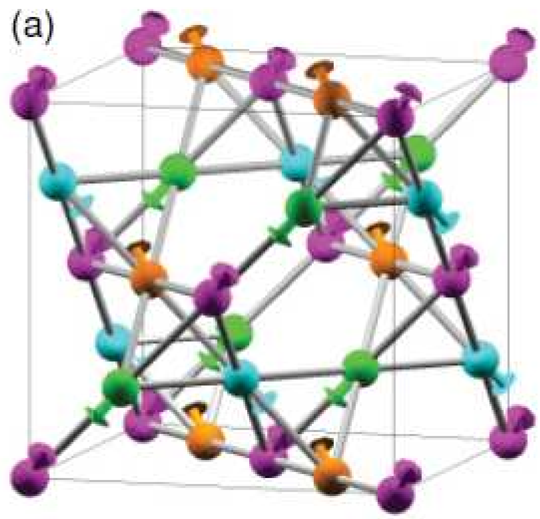
Correlated topological phase !

Phase diagram

LDA+U calc. Wan, Vishwanath, Savrasov

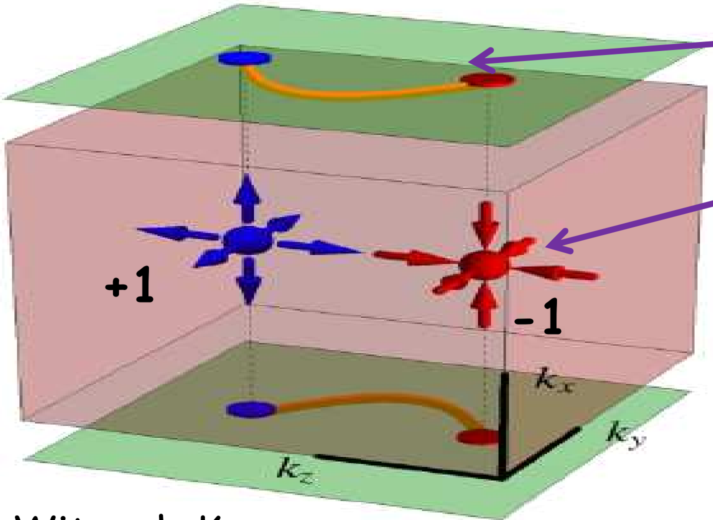


All-in/all-out AFM



Dirac semi-metal (or Weyl semi-metal) : Topological Metal

What is the (topological) Weyl semi-metal?



Witczak-Krempa

- Surface states : Fermi Arc
- Topological invariant
  : chiral charge

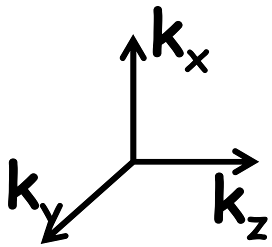
$$\boxed{C = \frac{\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3)}{|\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3)|} = \pm 1}$$

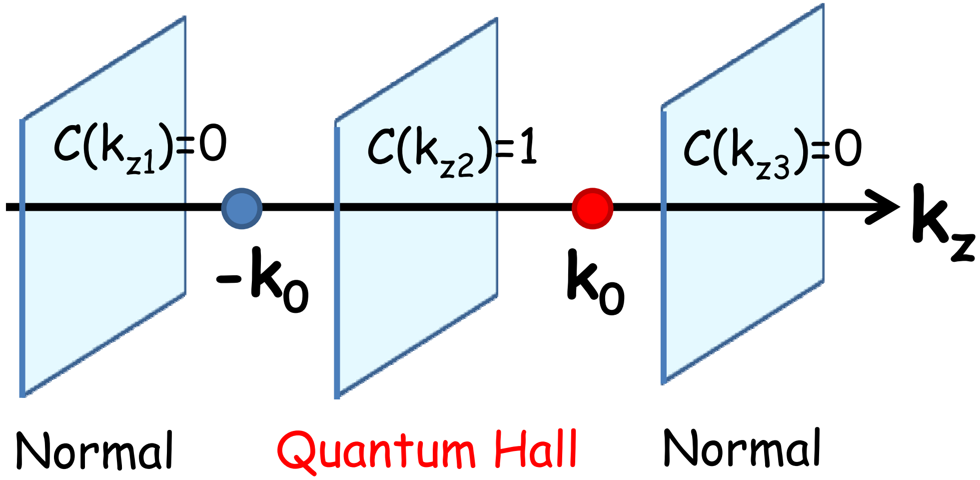
"Weyl fermion"

$$H(\mathbf{k}) = (v_1 \cdot k)\sigma_x + (v_2 \cdot k)\,\sigma_y + (v_3 \cdot k)\,\sigma_z$$

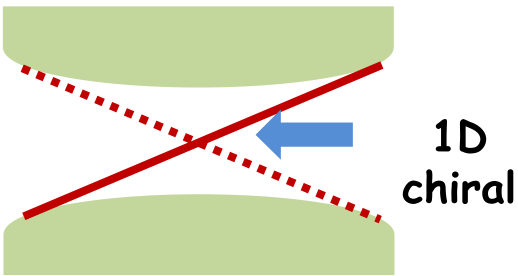
Quantum Hall effect of Weyl semi-metal

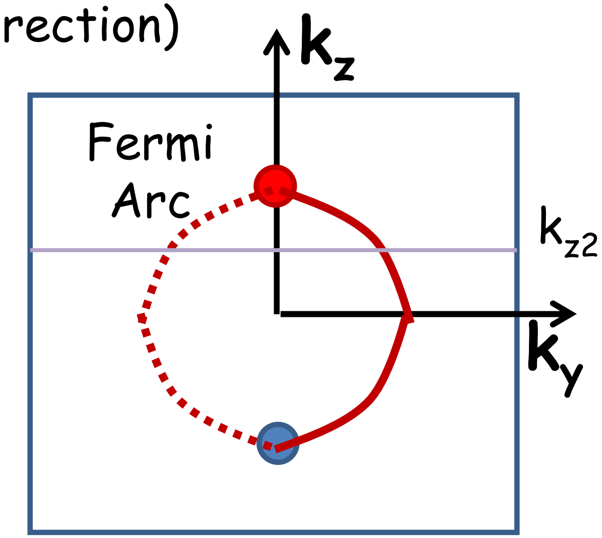
$$H(\mathbf{k}) = H_{kz}(k_x, k_y) = k_x\sigma_x + k_y\sigma_y + m\sigma_z, \quad m = (k_z - k_0)$$





- Surface spectrum (finite size along x-direction)



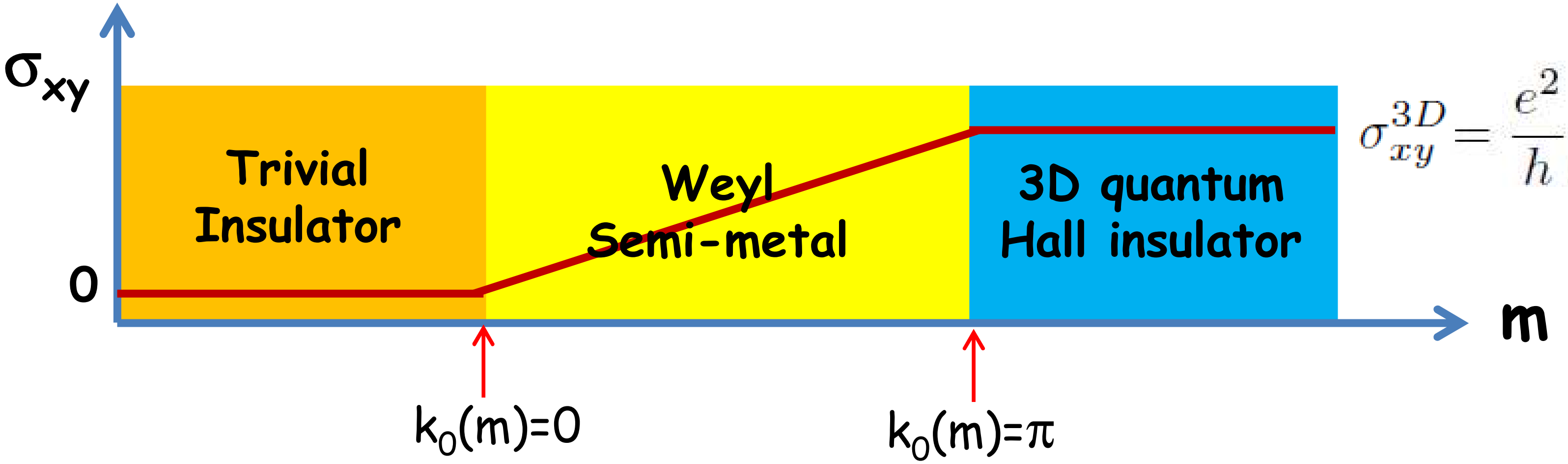


- Surface metallic states exist !
- Each Weyl point has a topological charge ± 1

Hall conductivity (σ_{xy}) in Weyl semi-metal

$$\sigma_{xy}^{3D,\mathrm{Weyl}} = \int_{-k_0}^{k_0} \frac{dk_z}{2\pi} \sigma_{xy}^{2D}(k_z) = \frac{e^2}{h} \frac{2k_0}{2\pi},$$

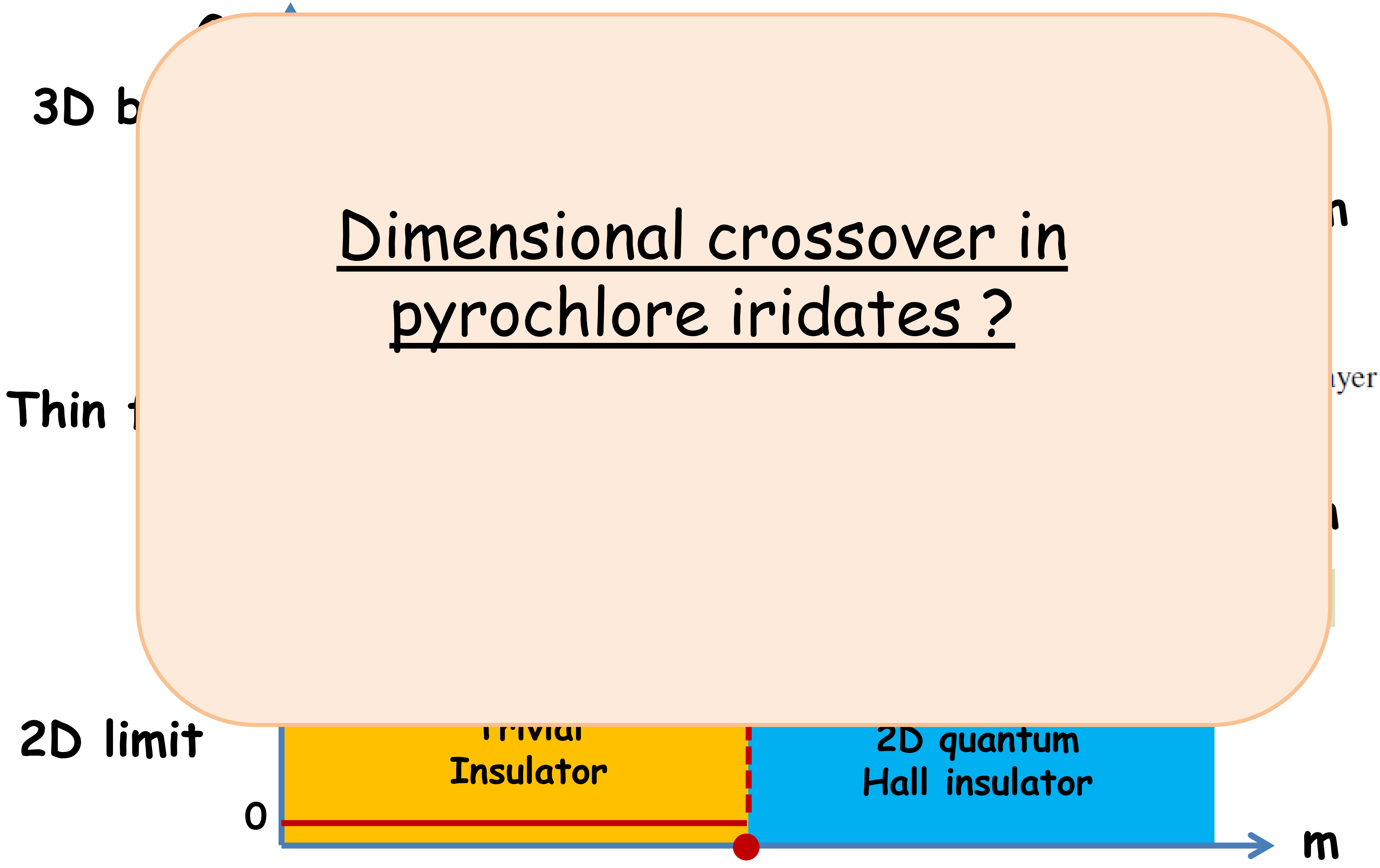
If $k_0=k_0(m)$



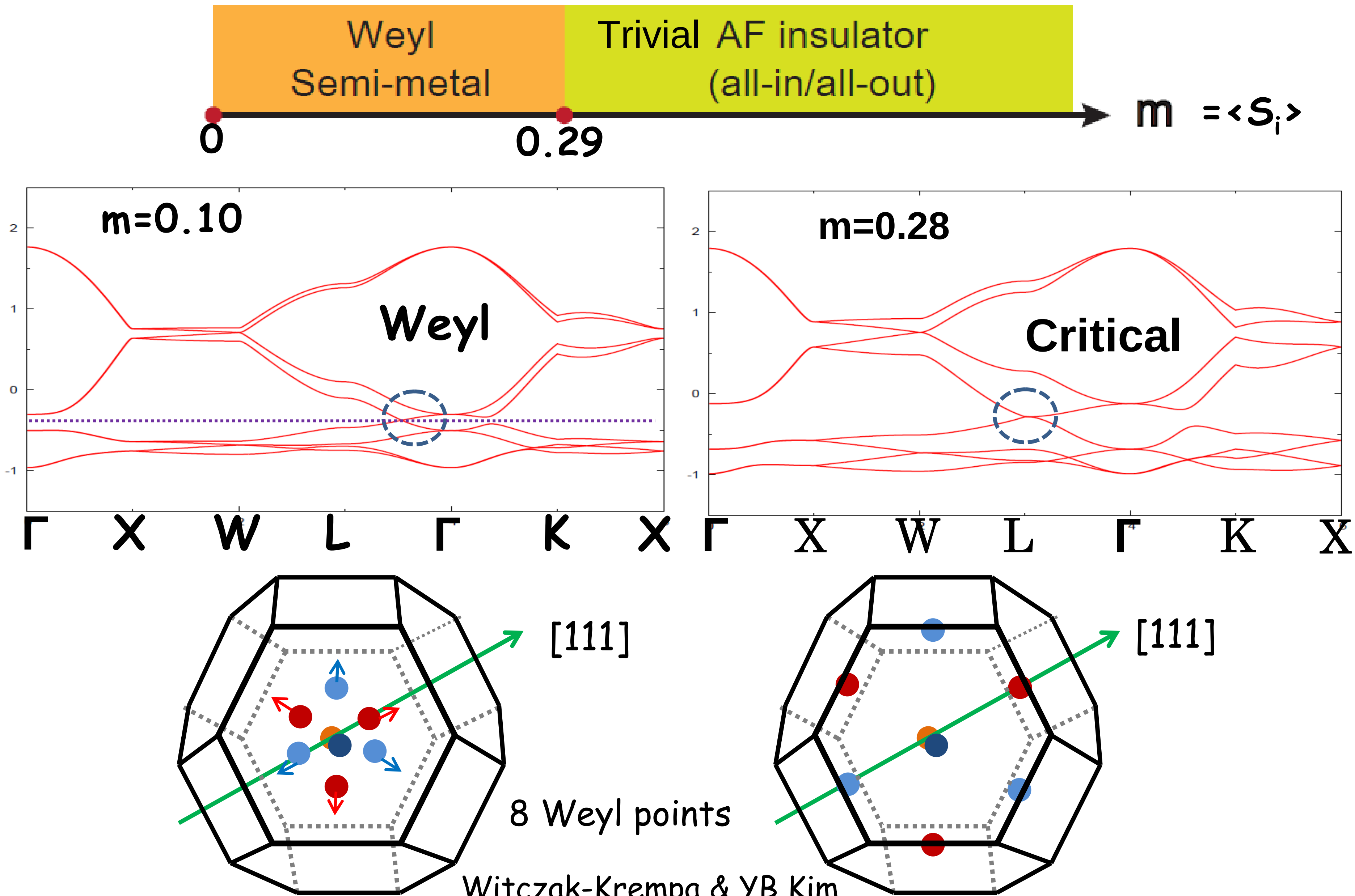
$$\sigma_{xy}^{3D} = \frac{e^2}{h} \frac{1}{a_z}$$

Dimensional crossover in Weyl semi-metal

Dimensional crossover in pyrochlore iridates ?



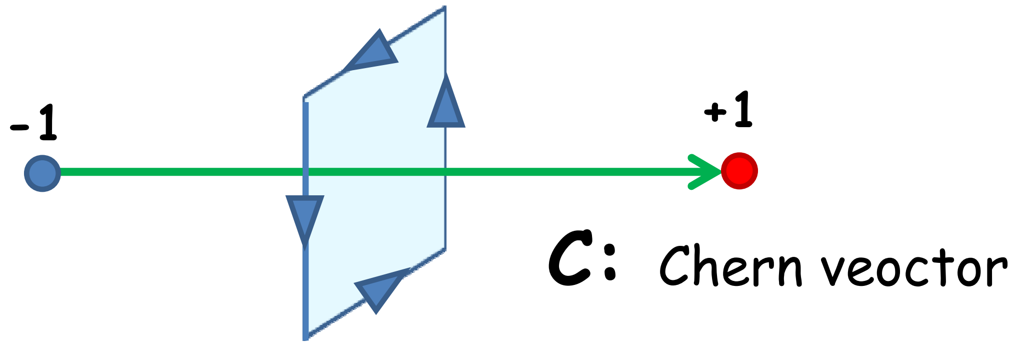
3D bulk phase diagram of iridates



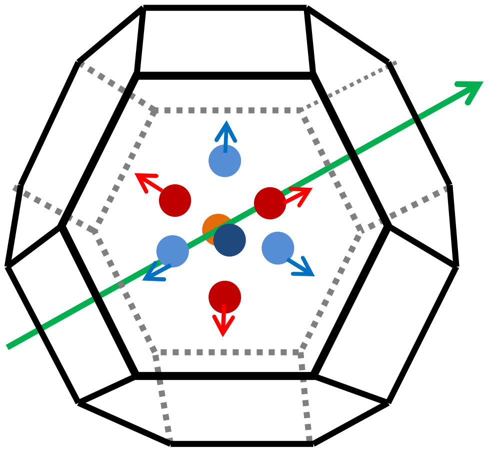
Witczak-Krempa & YB Kim

Chern vectors and cubic symmetry

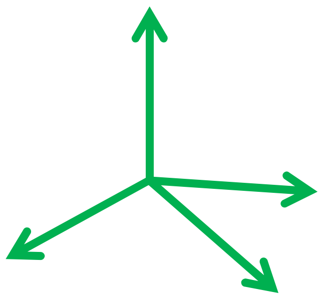
- For a pair of Weyl points



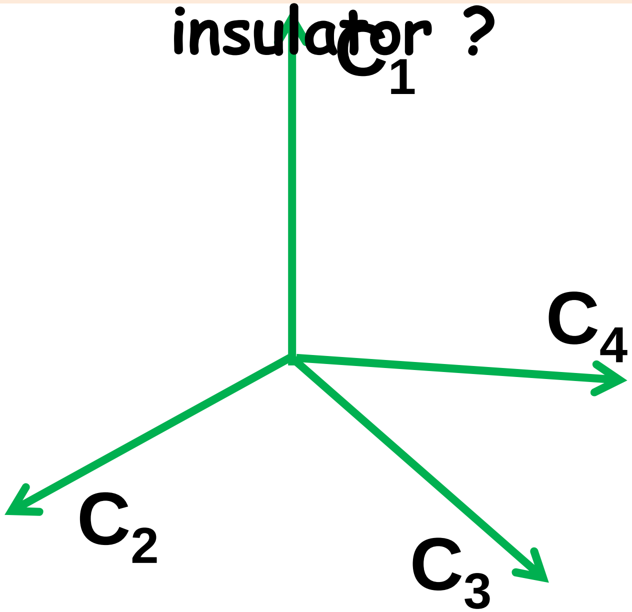
- Pyrochlore iridate
  :A system with multiple Weyl points (multiple Chern vectors)



Weyl semi-metal

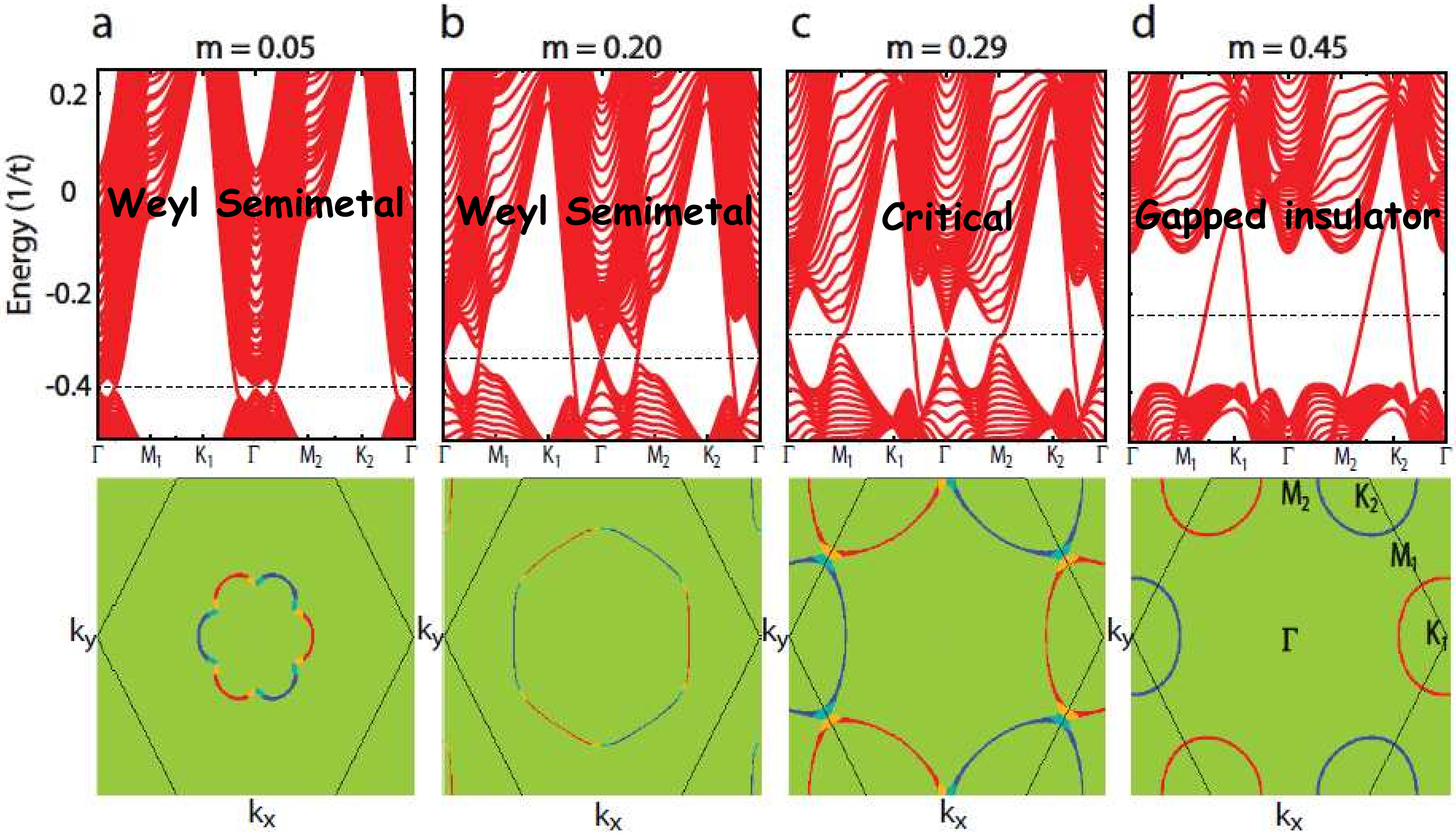


Anti-Chern insulator ?



$C_1+C_2+C_3+C_4=0$ due to cubic symmetry !

[111] Surface states



- At the critical point, the Fermi surface shows Lifshitz transition
- Fully-gapped insulator has surface states at the Fermi energy (Stable ?)

Pyrochlore iridate thin film

- Two main questions

1. Dimensional crossover in a system with multiple Weyl points

cf) A 3D Chern insulator with one pair of Weyl points

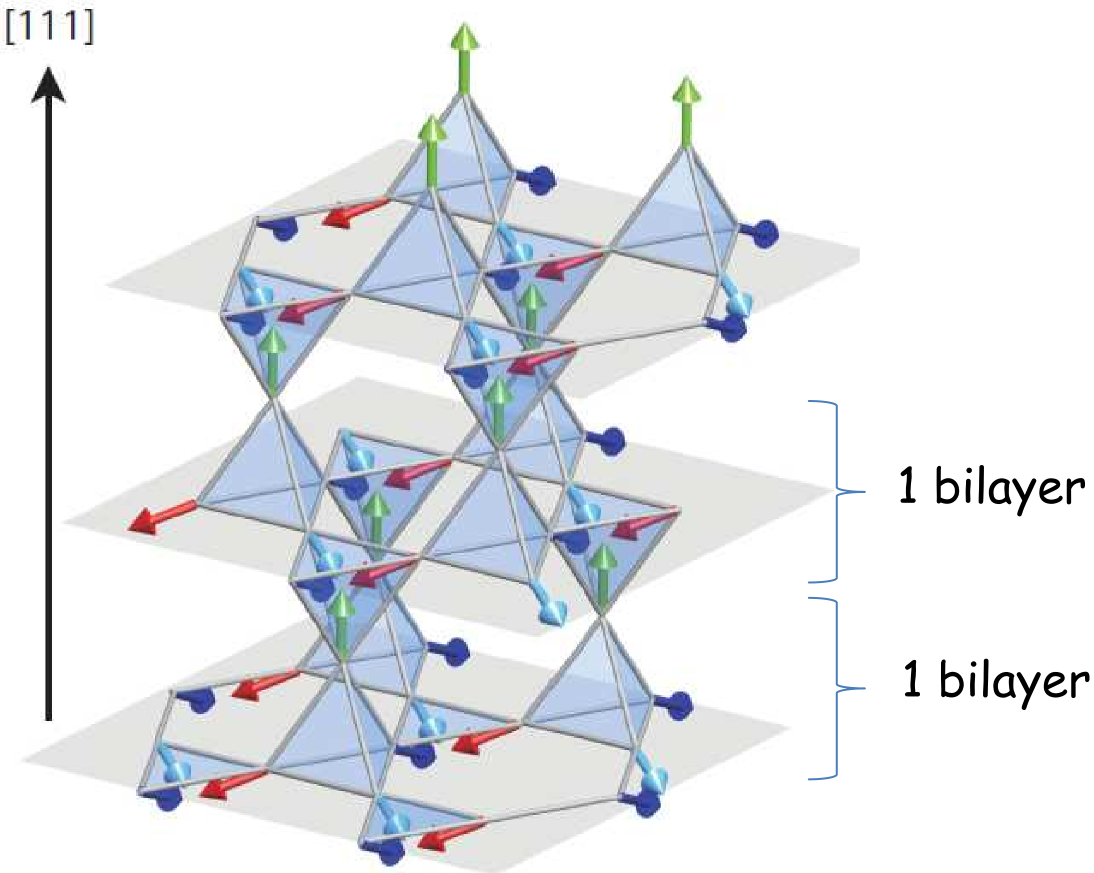
2. Fully-gapped AF insulator with topological property?
   Anti-Chern insulator ?

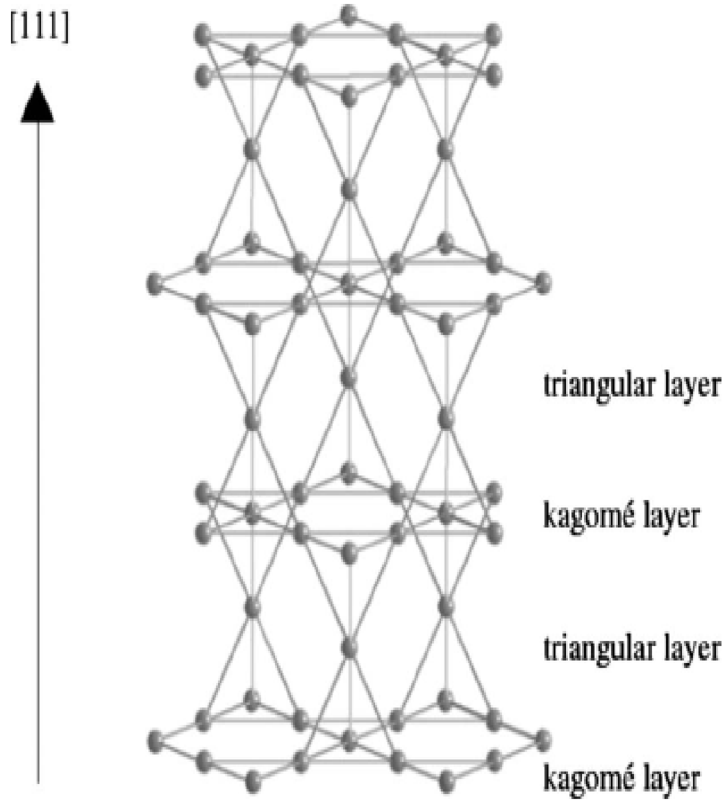
Weyl semi-metal in pyrochlore iridates

- Model Hamiltonian

1. Use J=1/2 states as a basis
2. Assume all-in/all-out magnetic ground states
3. Tune the magnitude of local magnetic moment $m=\langle S_i \rangle$

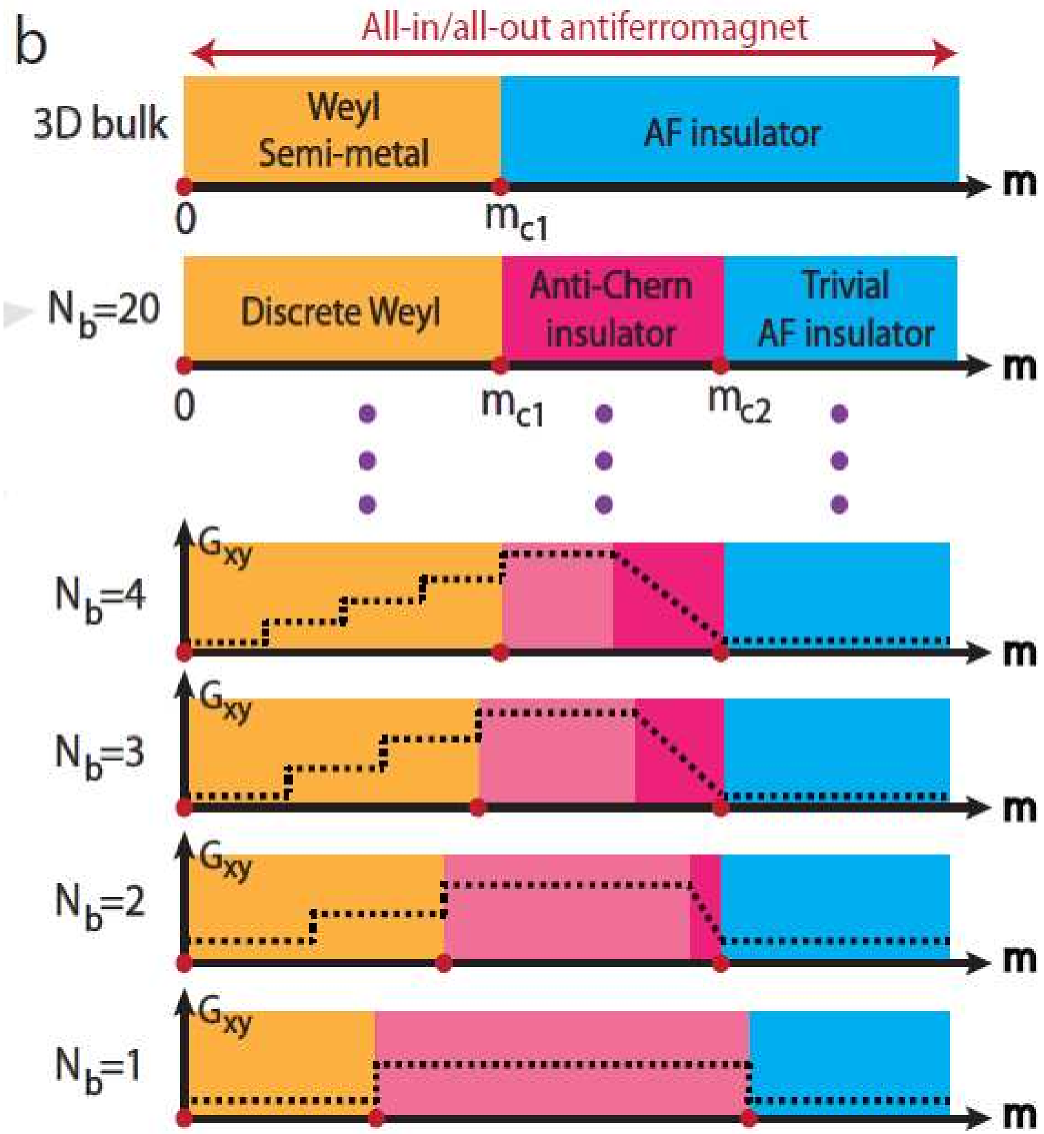
- [111] thin film : change the number of bilayers





Dimensional Crossover in [111] film

- G_{xy} ([111] // z-axis)

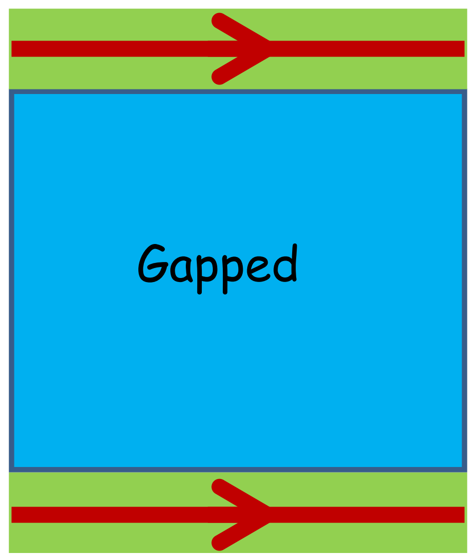


Rich physics in thin films !

1. Maximum $G_{xy} = \frac{e^2}{h} N_{layer}$

2. Anti-Chern insulator

- Bulk is gapped
- Surface states carry $G_{xy} \sim N_{layer}$



Surface Hall currents !

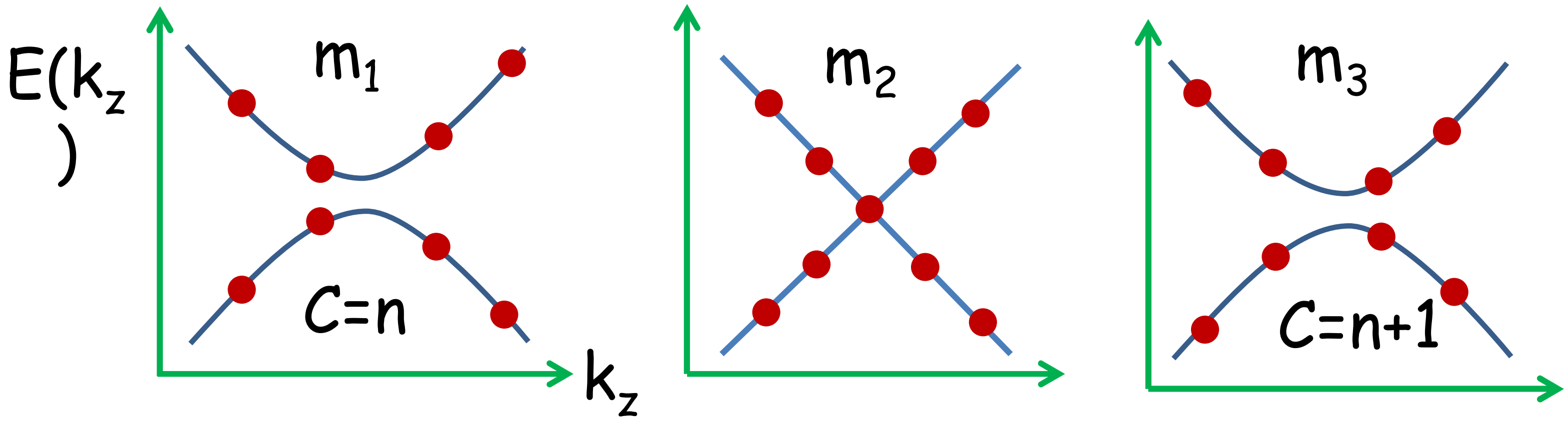
Accidental gap-closing at a Weyl point

Near a Weyl point : $H(\mathbf{k}) = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z$

In a film : k_z = discretized while k_x , k_y are good quantum number

Gap-closing is possible only when $k_x = k_y = k_z = 0$ simultaneously.

Accidental gap-closing is possible if $k_z = k_z(m) = 0$



$$E_+(k_z) = \frac{2\pi n}{L_z} + \frac{\varphi(m)}{L_z}$$

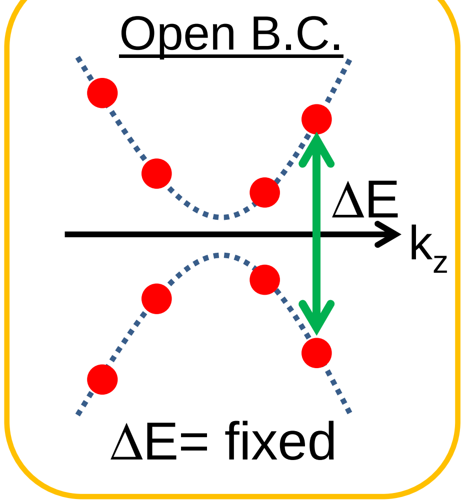
$$E_-(k_z) = -\frac{2\pi n}{L_z} - \frac{\varphi(m)}{L_z}$$

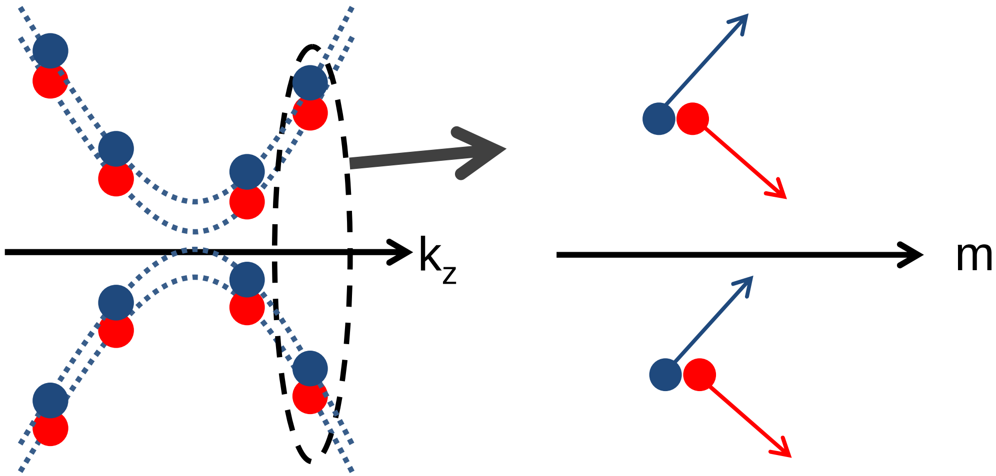
Gap-closing is possible whenever $\varphi(m) = -2\pi n$

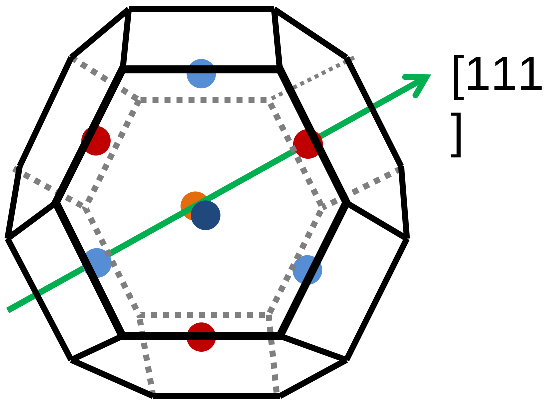
Open boundary condition

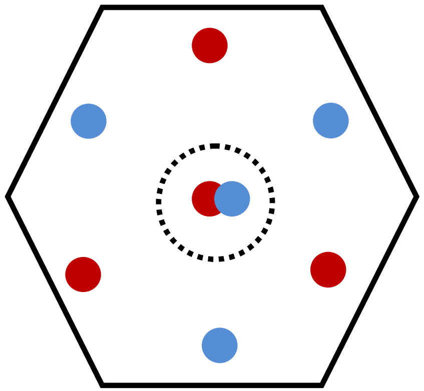
$$E_+(k_z) = \frac{2\pi(n+\frac{1}{2})}{L_z} + \frac{\varphi(m)}{L_z} \qquad E_-(k_z) = -\frac{2\pi(n+\frac{1}{2})}{L_z} + \frac{\varphi(m)}{L_z}$$

No gap-closing at a single Weyl point. Two coupled Weyl points required !

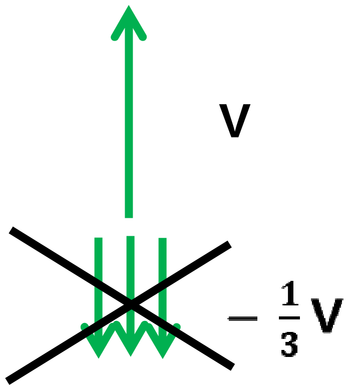




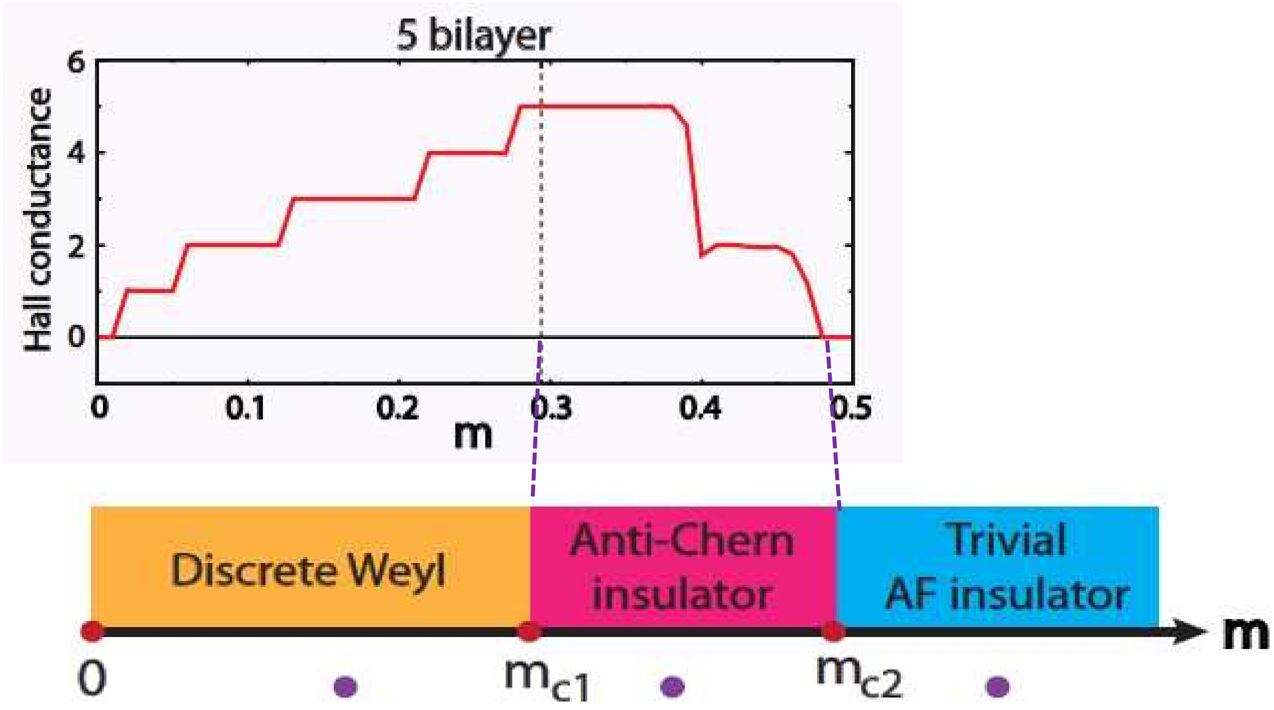




Surface Brillouin zone



How to release the Hall currents ?

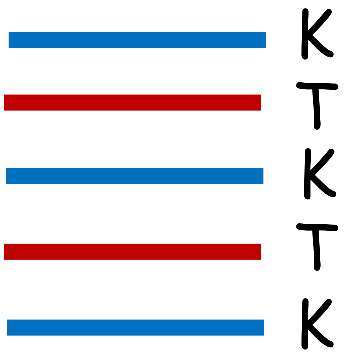


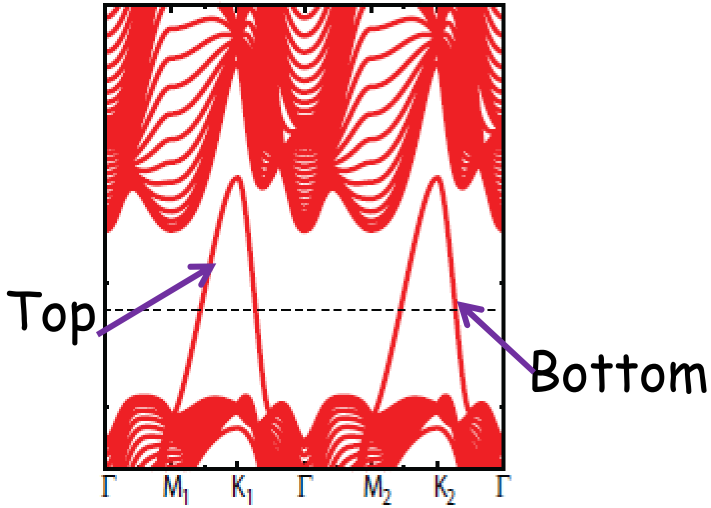
- Surface states mediated topological phase transition

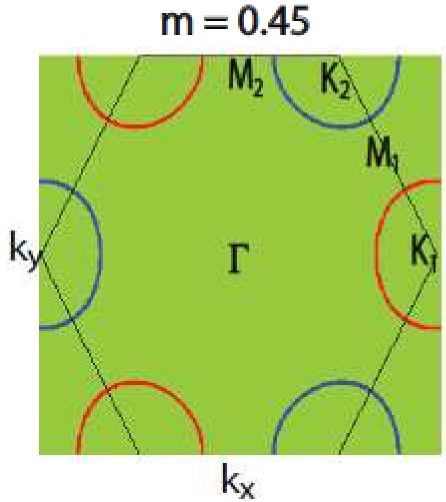
1. Surface states of anti-Chern insulator
2. Frustrated lattice geometry induced surface states

Surface states of anti-Chern insulator

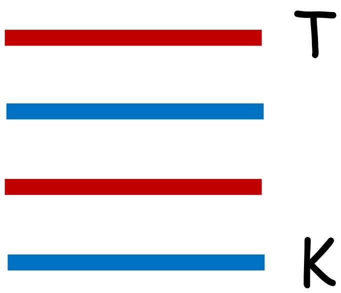
(1) KK film

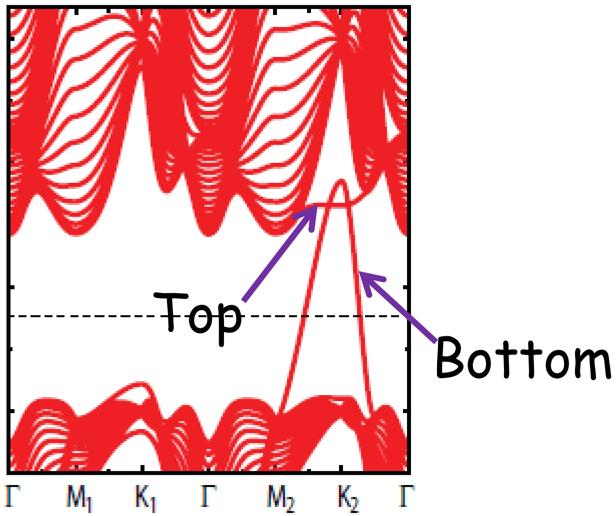


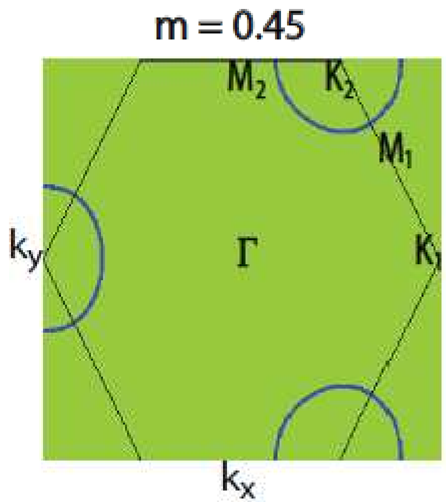




(2) KT film



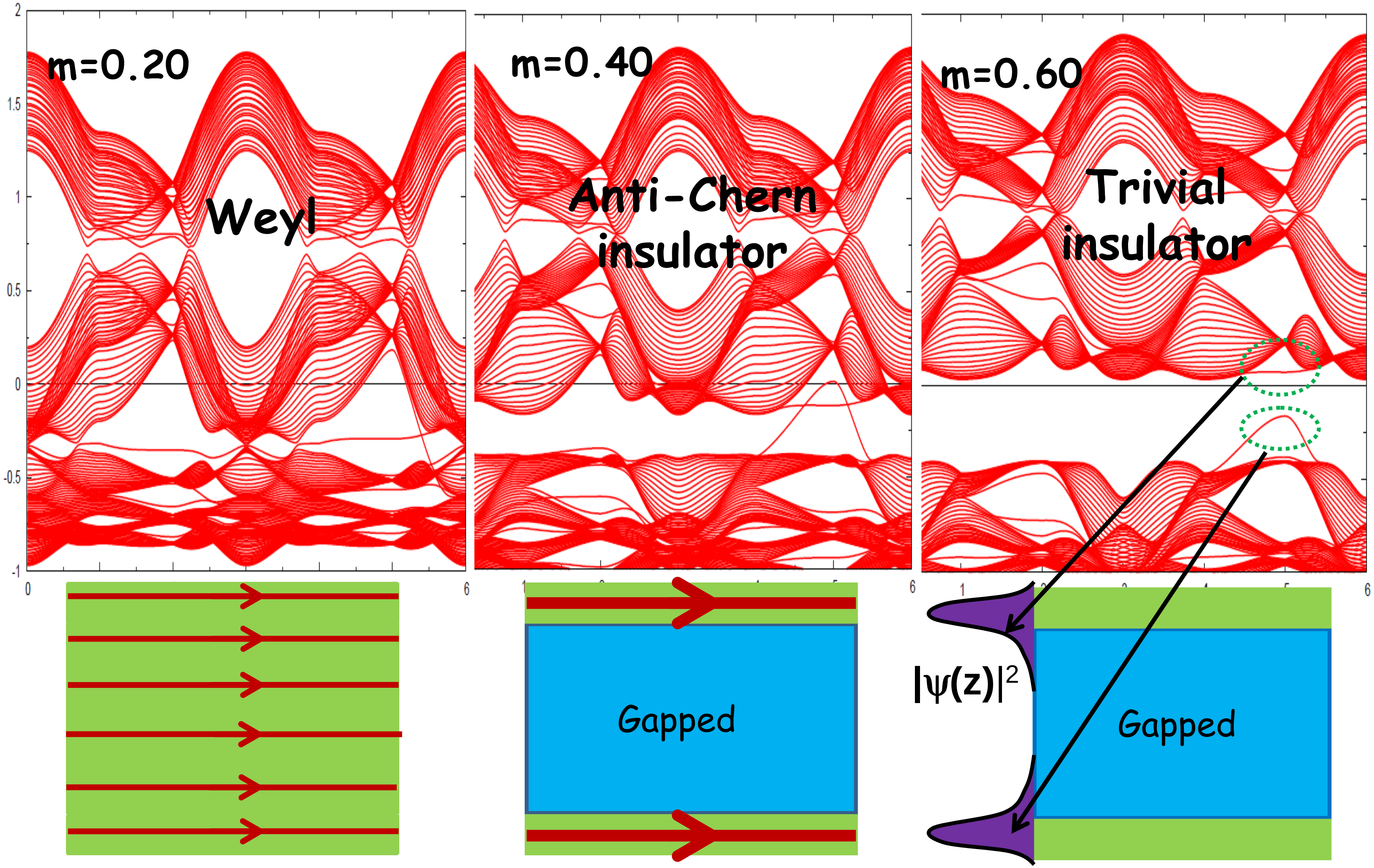




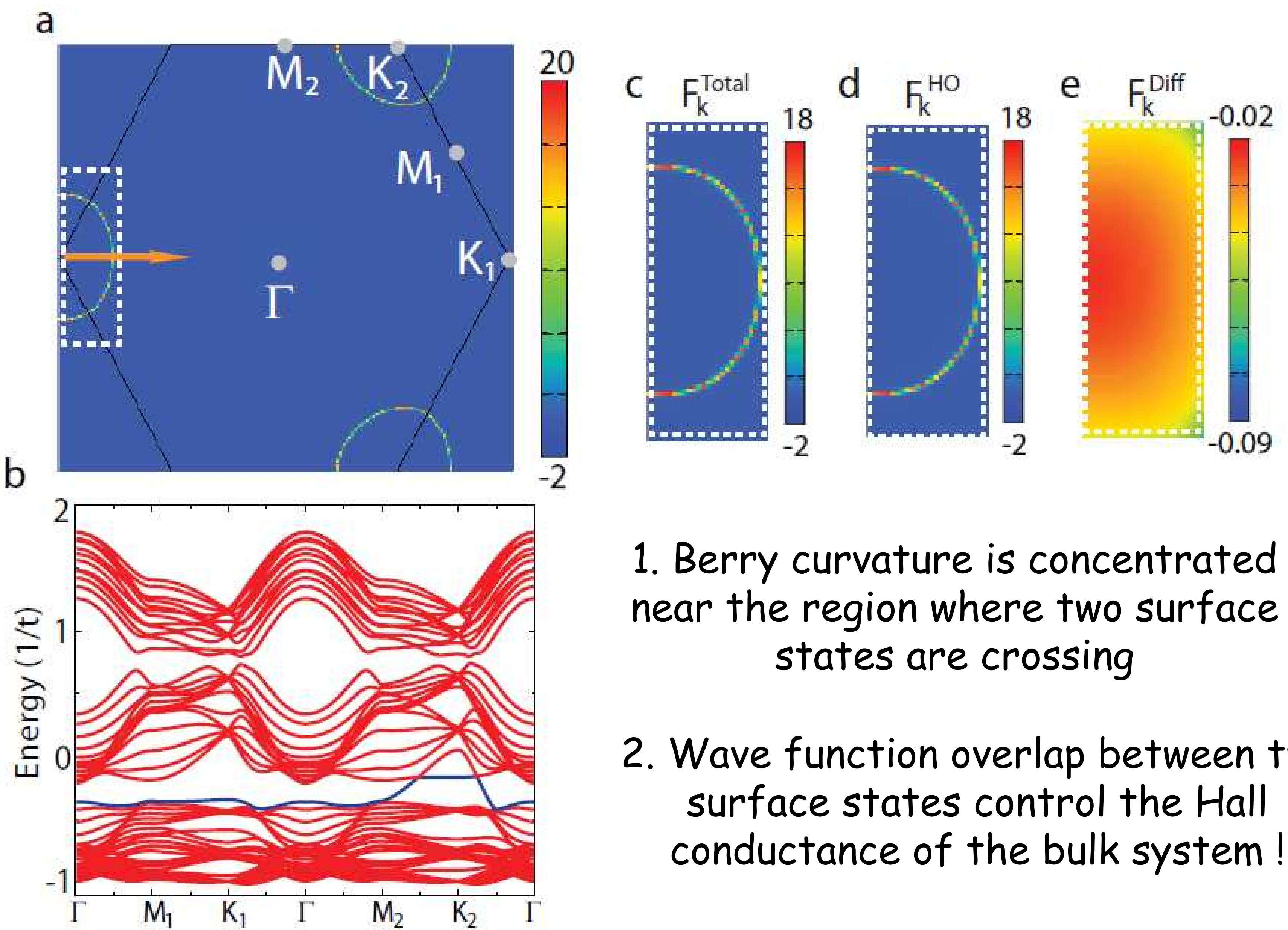
On the surface terminated by T layer there is additional geometrical surface states !

Anti-Chern insulator

- A new topological phase induced by surface states



Berry curvature distribution



1. Berry curvature is concentrated near the region where two surface states are crossing

2. Wave function overlap between two surface states control the Hall conductance of the bulk system !

Conclusion of part 2

Thin films of pyrochlore iridates have unexplored rich physics
(Dimensinal Crossover)

- Accidental band crossing in an intermediate dimension

⇒ Giant anomalous Hall effect in antiferromagnets

- Surface state induced topological phase transition

⇒ Anti-Chern insulator : a new phase existing only in thin films

Summary

Emergent topological phenomena in noncoplanar magnets

1. Surface quantum Hall effect

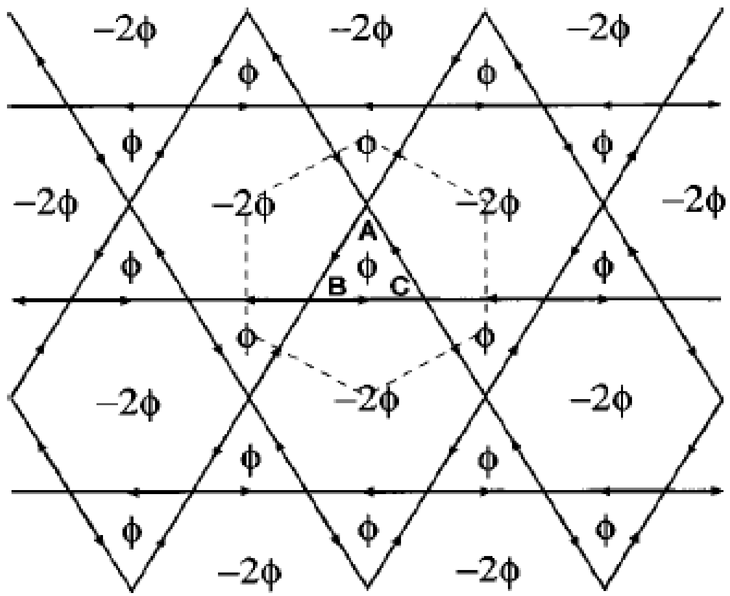
- Bound state in a continuum

2. Dimensional crossover in pyrochlore iridate thin films

- Modified accidental band crossing in thin films (Giant Hall currents)
- Surface states induced new topological phases (Anti-Chern insulator)

Quantum Hall effect in non-coplanar magnets

$$H=\sum_{NN} t_{ij}\psi^{\dagger}_{i\sigma}\psi_{j\sigma}-J_H\sum_{i} \psi^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_i\psi_{i\beta}\,,$$

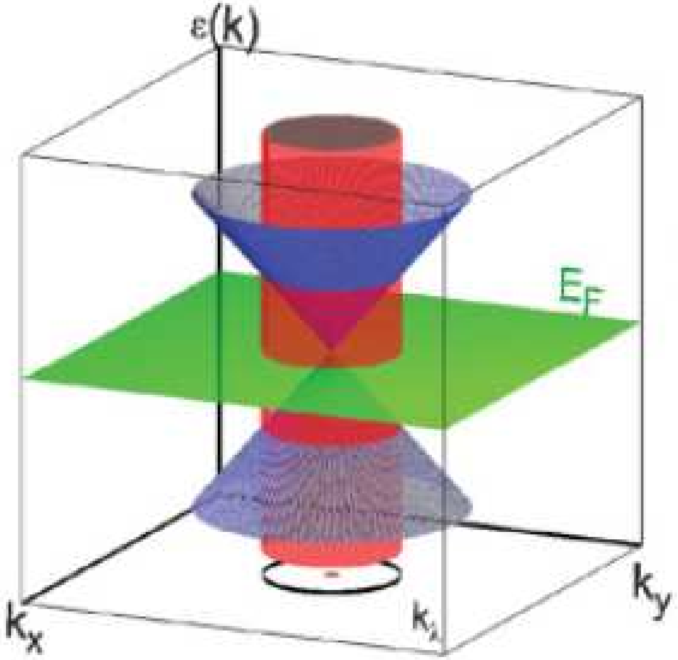


Ohgushi, Murakami, Nagaosa

Spin Berry phase can generate quantum Hall effects

Topological number of Weyl semi-metal

$$C = \frac{1}{2\pi}\int d\mathbf{k}\cdot\nabla\times\mathbf{A}(\mathbf{k}) \qquad \mathbf{A}(\mathbf{k}) = i\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle$$



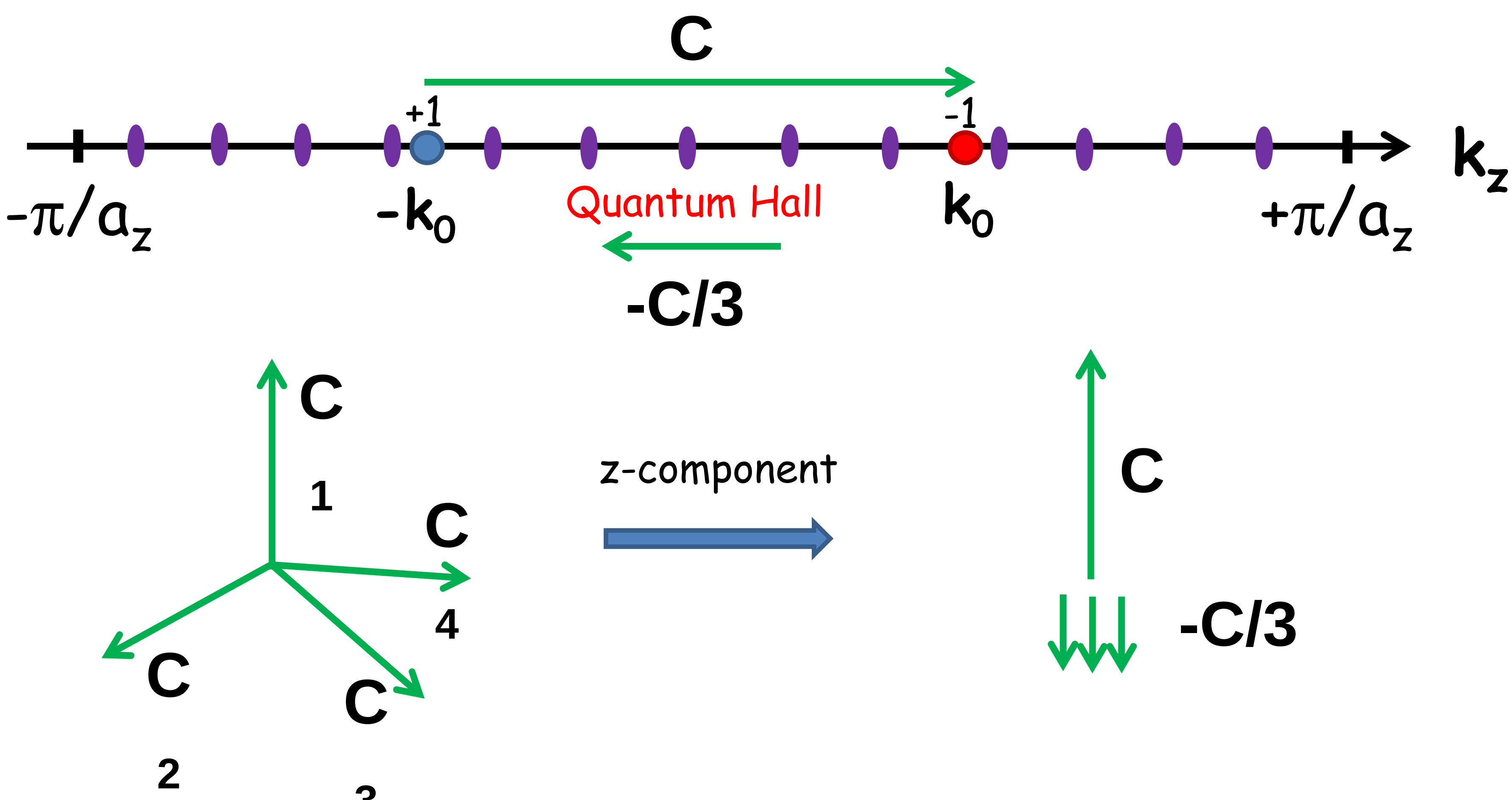
Wan et al., PRB

$$H = (\mathbf{v}_1\cdot\mathbf{k})\sigma_1 + (\mathbf{v}_2\cdot\mathbf{k})\sigma_2 + (\mathbf{v}_3\cdot\mathbf{k})\sigma_3$$

$$\boxed{C = \frac{\mathbf{v}_1\cdot(\mathbf{v}_2\times\mathbf{v}_3)}{|\mathbf{v}_1\cdot(\mathbf{v}_2\times\mathbf{v}_3)|} = \pm 1}$$

Weyl point has a topological number i.e., chiral charge !

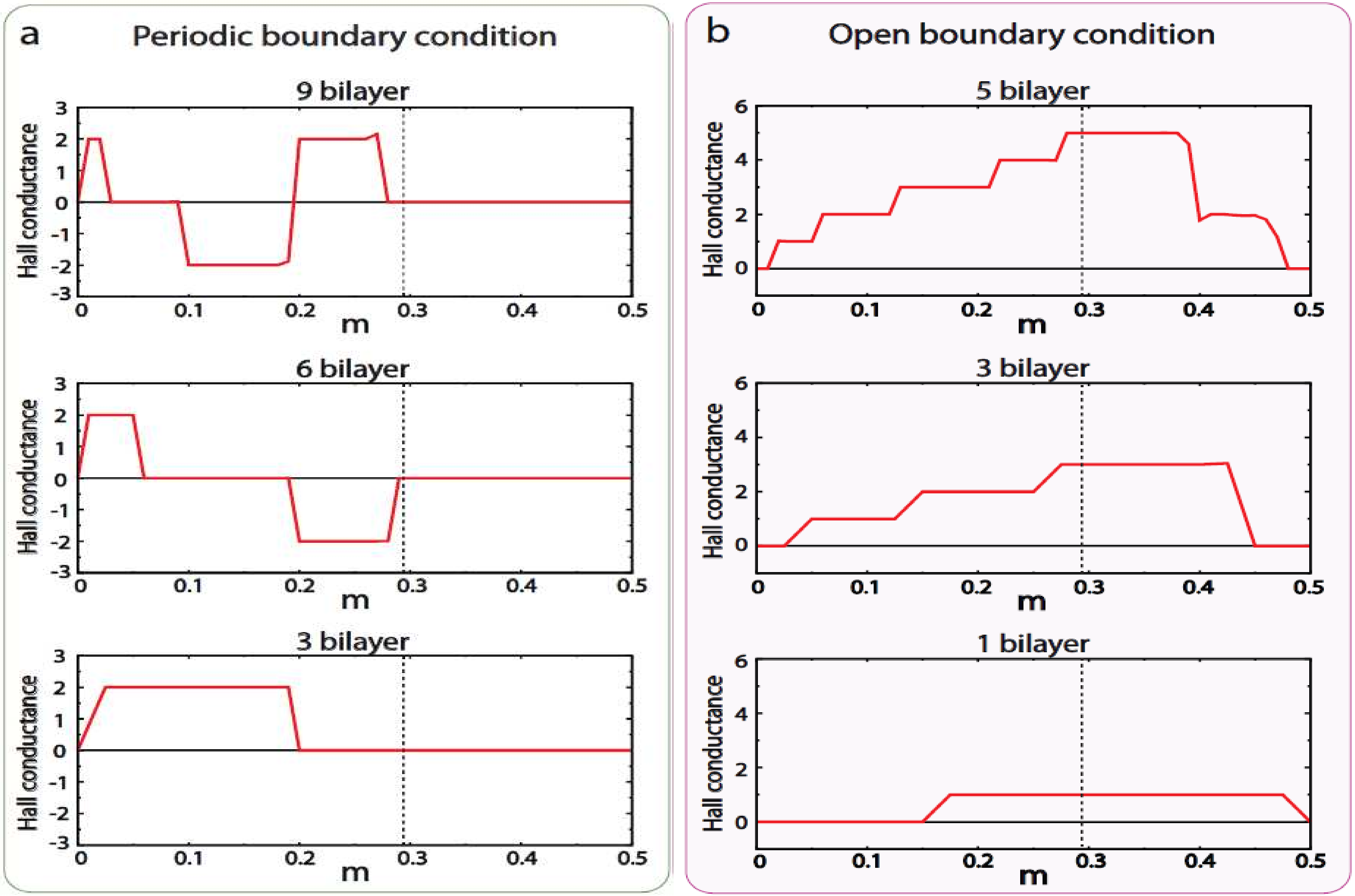
Finite size effect on Weyl semimetal



Number of discrete momenta in $[-k_0, k_0]$

$\neq$ 3×Number of discrete momenta in $[-k_0/3, k_0/3]$

Anomalous Hall conductance

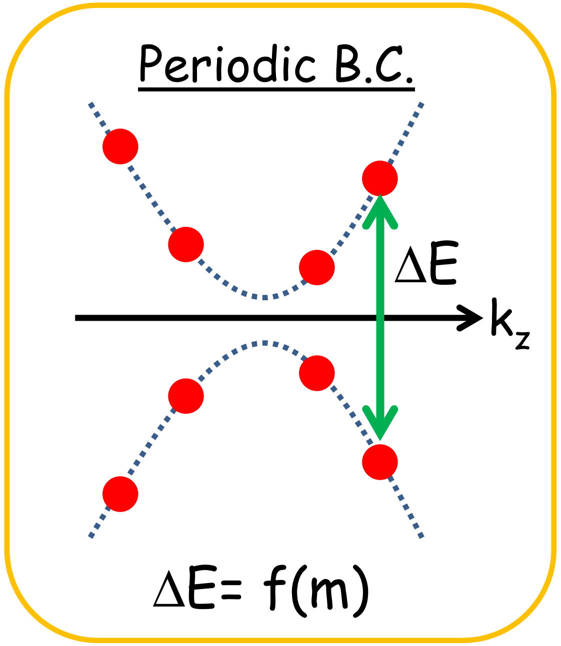


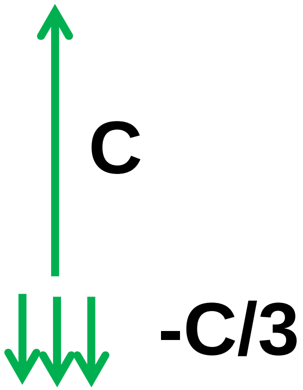
Periodic boundary condition

$$E_+(k_z)=\frac{2\pi n}{L_z}+\frac{\varphi(m)}{L_z} \quad E_-(k_z)=-\frac{2\pi n}{L_z}-\frac{\varphi(m)}{L_z}$$

$$\Phi(z+L_z/2)=\Phi(z-L_z/2), \quad \Phi(\mathbf{r})\sim e^{i\mathbf{k}_W\cdot\mathbf{r}}\psi(\mathbf{r})$$

$$\psi(z+L_z/2)=e^{i\phi}\psi(z-L_z/2) \text{ with } \phi=\phi(m)$$





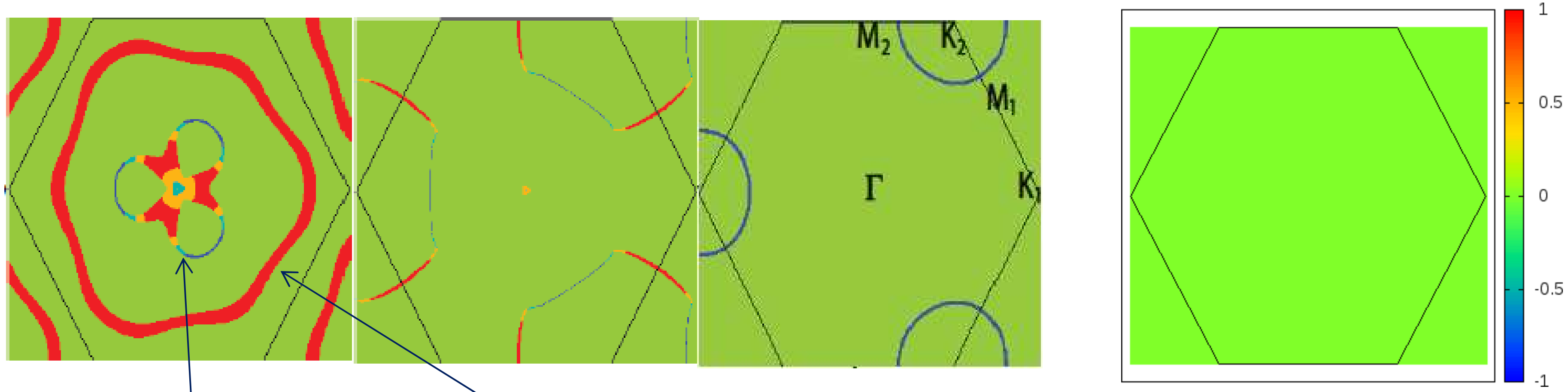
Accidental gap-closing is possible at all 8 Weyl points !

Layer resolved Fermi-surface: 20bilayer film

- Red (Blue) line : states localized on the top (bottom) surface

Weyl Semimetal | Anti-Chern insulator | Trivial AF

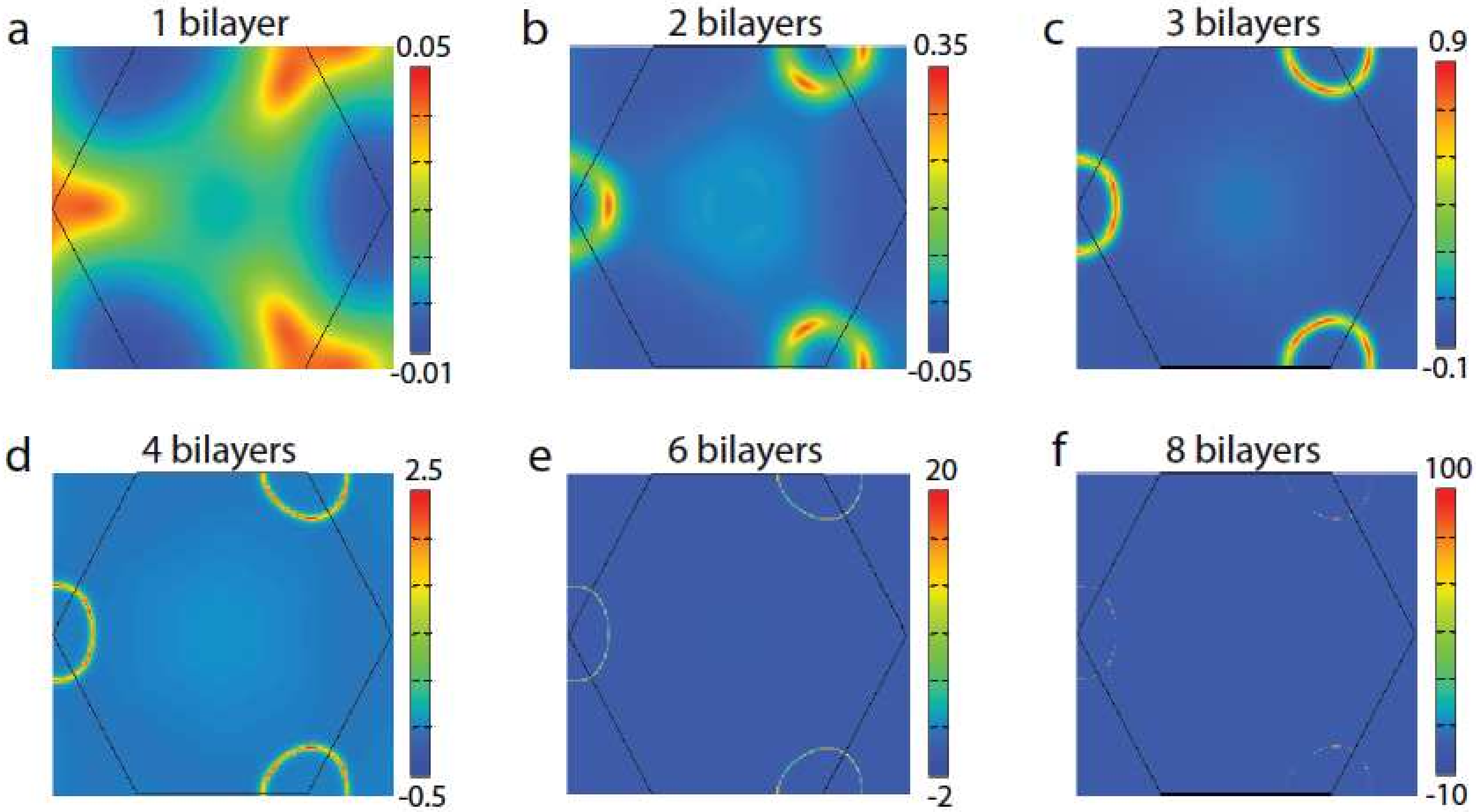
m=0.05 | m=0.15 | m=0.40 | m=1.0



Fermi Arc

Localized state due to lattice structure

Surface state mediated phase transition



Exponentially small overlap between two surfaces !