

Spin Hall and quantum spin Hall effects

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PRESTO, JST

Introduction – Spin Hall effect

spin Hall effect in Pt

Quantum spin Hall phase

2D

3D

phase transition from the ordinary insulator phase

Collaborators: N. Nagaosa, S.-C. Zhang, S. Iso, Y. Avishai,
M. Onoda, G. Y. Guo, T. W. Chen

Intrinsic spin Hall effect

effect

- p-type semiconductors

(SM, Nagaosa, Zhang, Science (2003))

Luttinger model

$$H = \frac{\hbar^2}{2m} \left[\left(\gamma_1 + \frac{5}{2} \gamma_2 \right) k^2 - 2\gamma_2 (\vec{k} \times \vec{S}) \right]$$

(\vec{S} : spin-3/2 matrix)

- 2D n-type semiconductors in heterostructure
- (Sinova et al., PRL (2004))

Rashba model

$$H = \frac{k^2}{2m} + \lambda (\vec{\sigma} \times \vec{k})_z$$

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-
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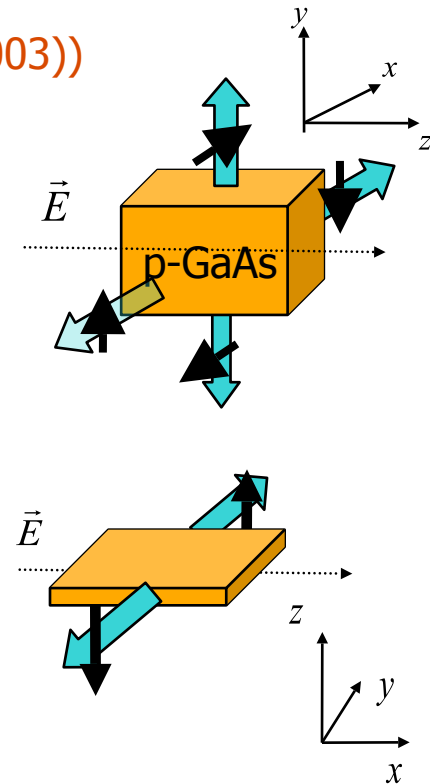
$$j_j^i = \sigma_s \varepsilon_{ijk} E_k \quad \left\{ \begin{array}{l} i: \text{spin direction} \\ j: \text{current direction} \\ k: \text{electric field} \end{array} \right.$$

σ_s : even under time reversal

$$j_j^i \approx S^i v_j \quad \bullet \text{ Nonzero in nonmagnetic materials.}$$

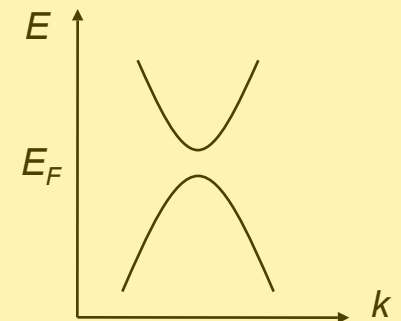
Cf. Extrinsic spin Hall effect

← impurity scattering



Berry phase in k-space

← band crossing



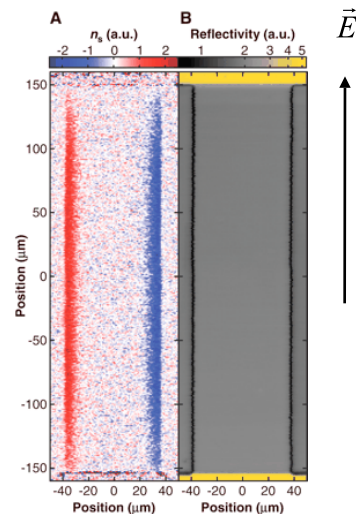
Experiments on spin Hall effect

• 3D n-type, Kerr rotation

- Y.K.Kato, R.C.Myers, A.C.Gossard, D.D. Awschalom, Science (2004)
- Sih et al. , Nature Phys. (2005)
- Sih et al., PRL (2006)
- Stern et al., PRL(2006) n-ZnSe

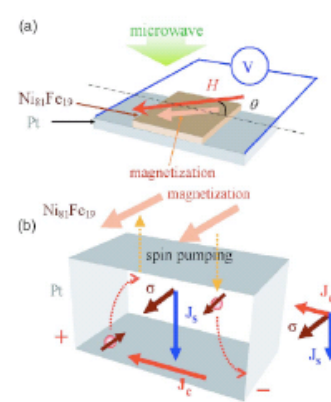
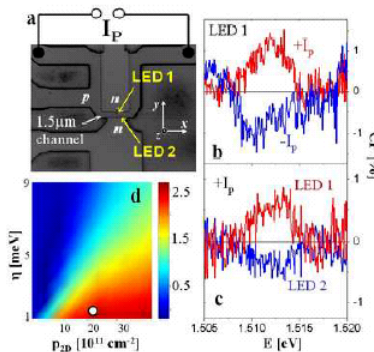
n-GaAs, n- (In,Ga)As

RT



• 2D p-type, spin LED

- J. Wunderlich et al., PRL(2005)
- p-GaAs



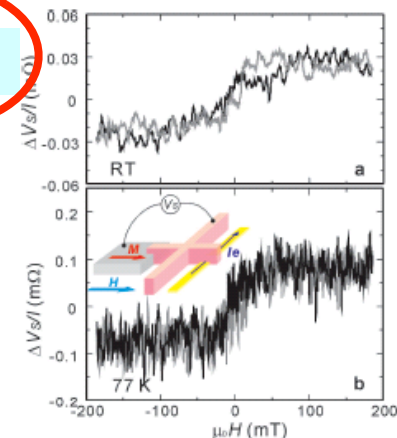
• Metal (Pt, Al) -- Inverse SHE

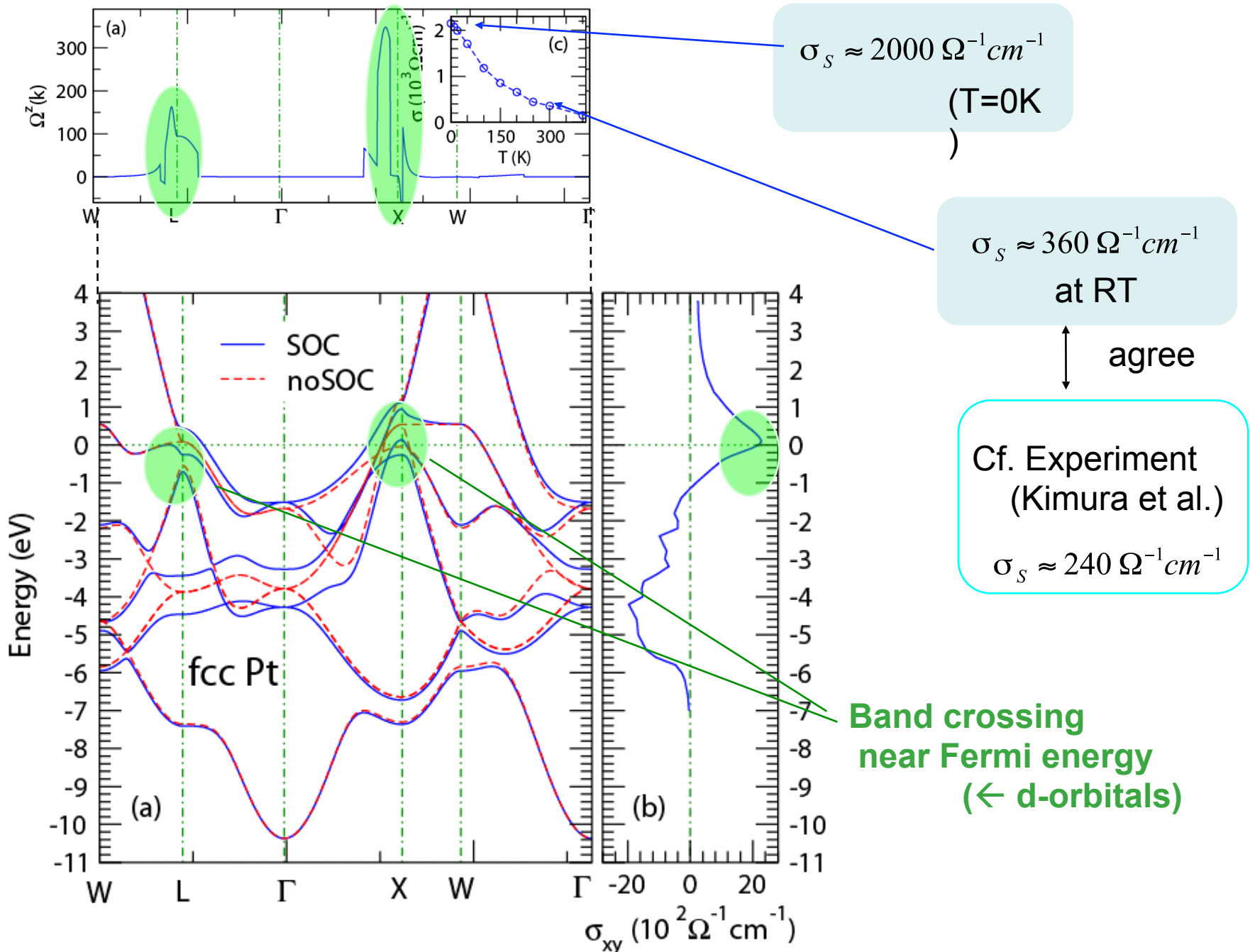
- E. Saitoh, M. Ueda, H. Miyajima, G. Tatara, APL (2006)
- Valenzuela and Tinkham, Nature(2006) Al

Pt RT

• Metal (Pt) -- SHE & Inverse SHE

- T. Kimura, Y. Otani, T. Sato, S. Takahashi, S. Maekawa, PRL (2007) Pt RT





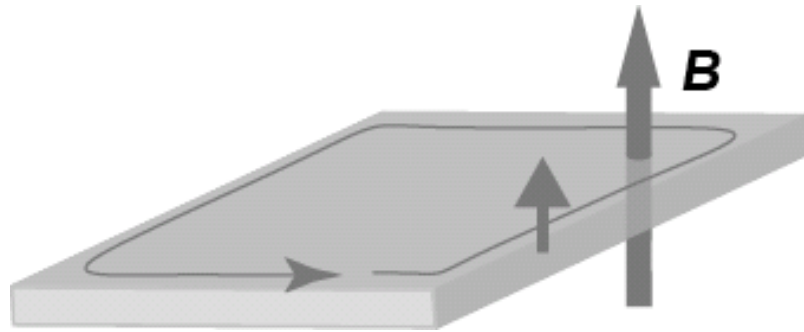
2D quantum spin Hall phase

Quantum spin Hall phases

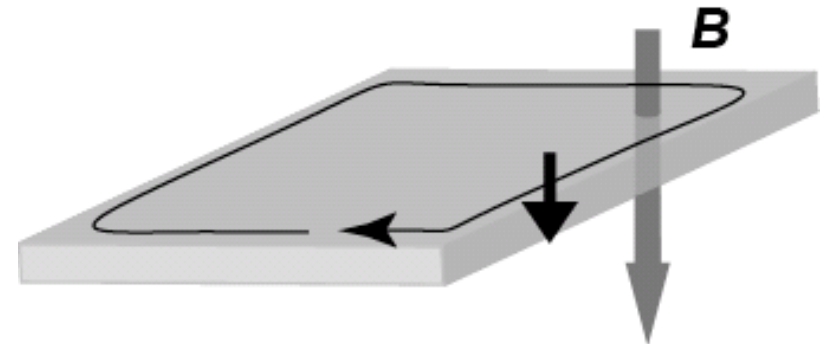
Bernevig and Zhang, PRL (2005)
Kane and Mele, PRL (2005),

- bulk = gapped (insulator)
- gapless edge states -- carry spin current, topologically protected

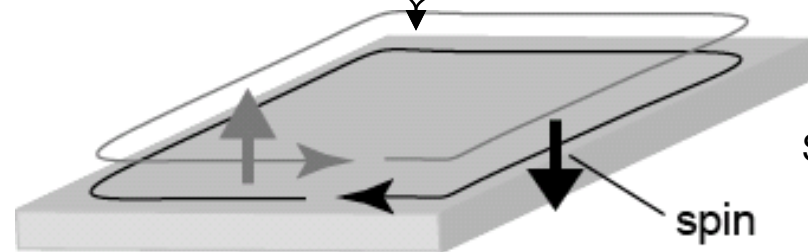
Quantum spin Hall state \approx Quantum Hall state $\times 2$



$$\sigma_{xy} = \frac{e^2}{h} \text{ for up spin}$$



$$\sigma_{xy} = -\frac{e^2}{h} \text{ for down spin}$$



Spin-orbit coupling
 \rightarrow (spin-dependent) effective magnetic field

Z_2 topological number ν

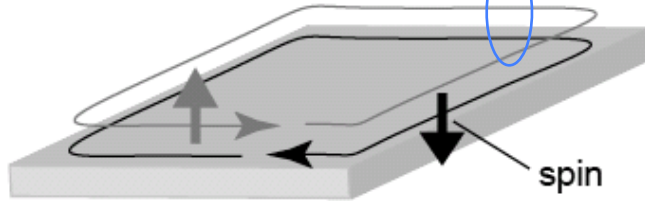
Even \rightarrow simple insulator

Odd \rightarrow quantum spin Hall phase

Kane and Mele, PRL95, 146802
(2005)

(i) Quantum spin Hall phase ($\nu = \text{odd}$)

no backscattering by nonmagnetic impurities.



Odd number of Kramers pairs of edge states

Edge states

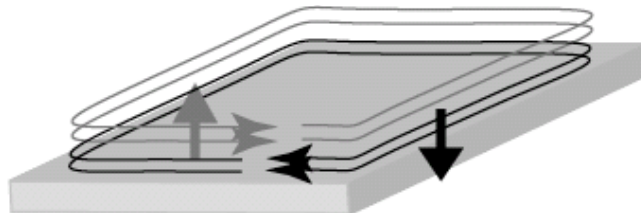
\rightarrow robust against { nonmagnetic impurities
interaction

Wu, Bernevig, Zhang, PRL (2006)

Xu, Moore, PRB (2006)

(ii) Simple insulator ν

(



Even number of Kramers pairs of edge states

\approx

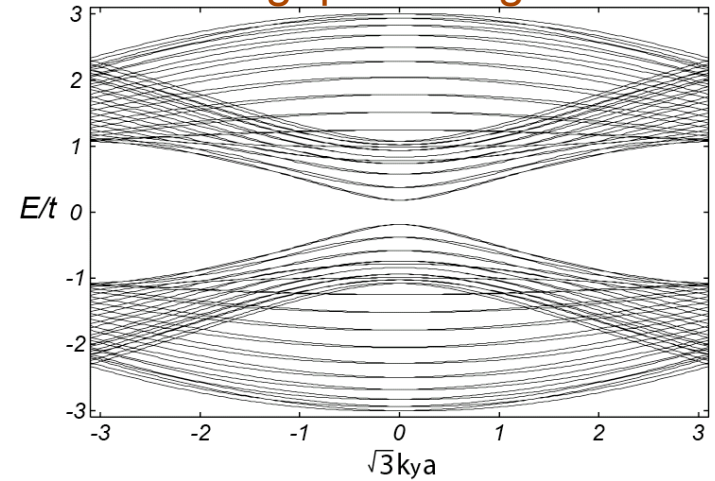
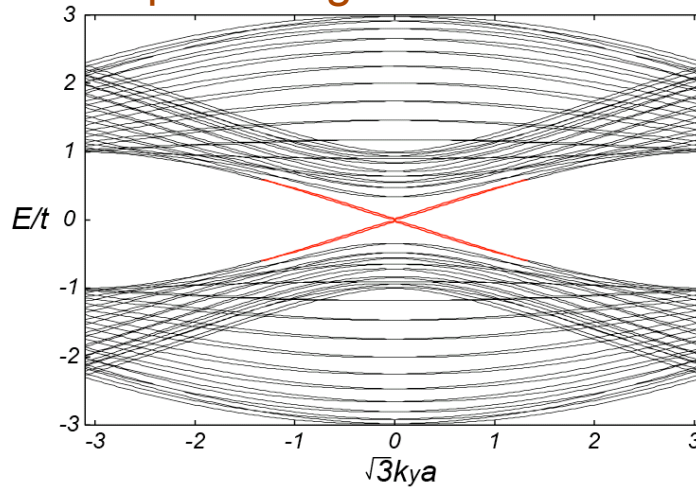
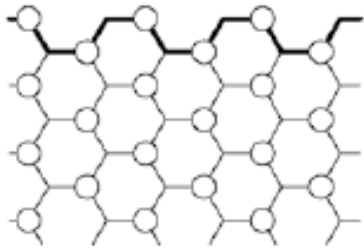


Kane-Mele model

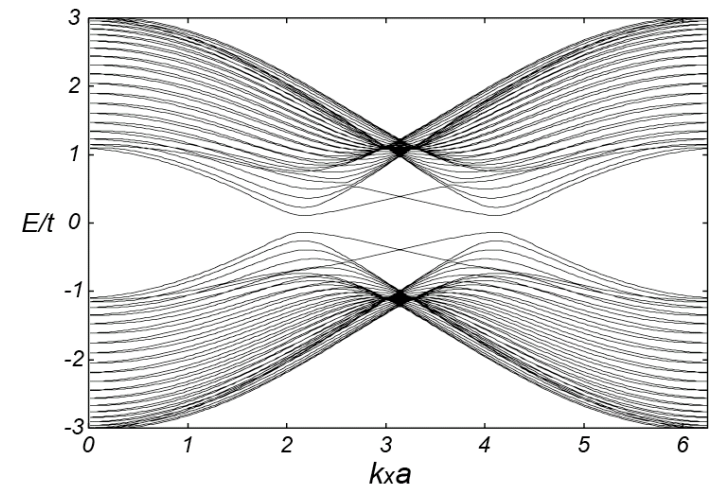
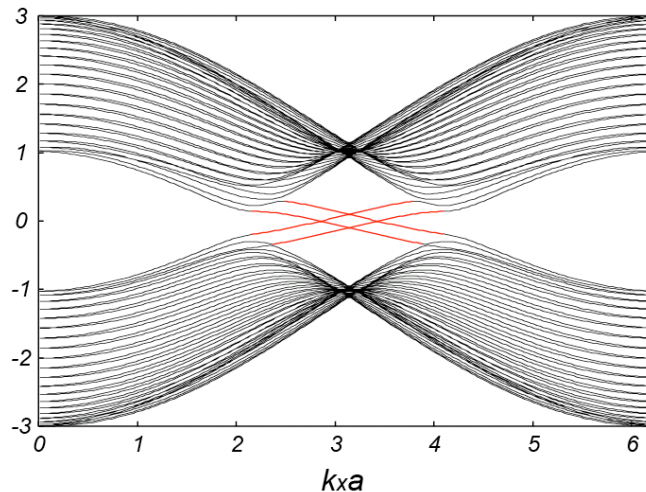
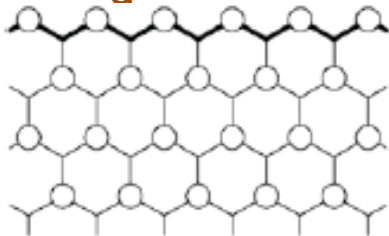
Quantum spin Hall phase ($\nu = \text{odd}$)
→ Gapless edge states

Simple insulator ($\nu = \text{even}$)
→ No gapless edge states

armchair



zigzag



**Gapless edge states exist irrespective of boundary conditions
topologically protected**

Bulk topological order → manifest as edge states

In contrast : Graphene without spin-orbit → Edge states only on zigzag edges

Z_2 topological number is a bulk property

Z_2 topological number in 2D systems **without** inversion-symmetry

Fu, Kane, PRB74,195312('06)

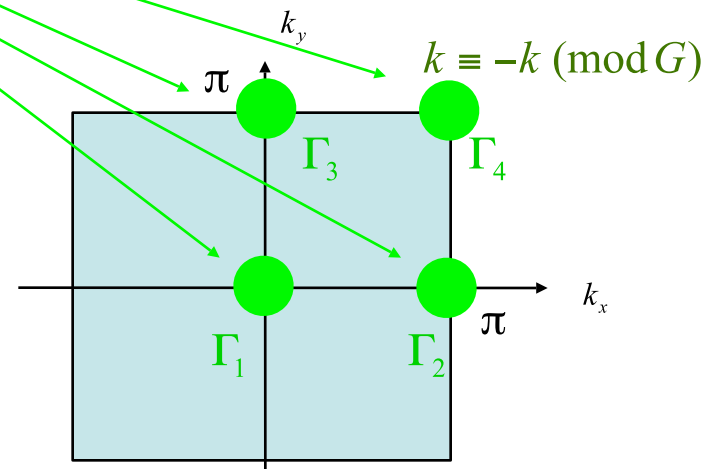
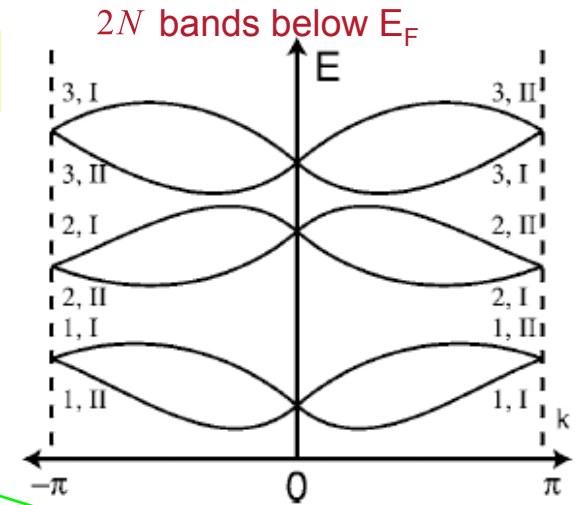
$$w_{mn}(\vec{k}) = \langle u_{-k,m} | \Theta | u_{k,n} \rangle \quad 2N \times 2N \text{ unitary}$$

(& antisymmetric at $\Gamma_i = \frac{1}{2} \vec{G}$)

Z_2 topological number ν

$$(-1)^\nu = \prod_{i=1}^4 \frac{\sqrt{\det[w(\Gamma_i)]}}{\text{Pf}[w(\Gamma_i)]}$$

$= \pm 1$ -- Choice of branches of $\pm \sqrt{\det[w(\Gamma_i)]}$



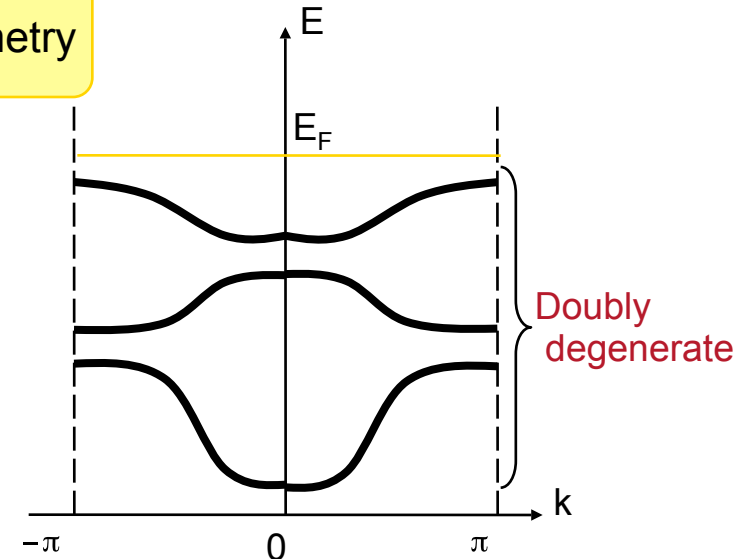
No inversion symmetry

→ Phases of the wavefunctions should be calculated for the whole BZ

Z_2 topological number in 2D systems with inversion-symmetry

Fu, Kane, PRB76, 045302 (2007)

$2N$ bands below E_F (N Kramers pairs)

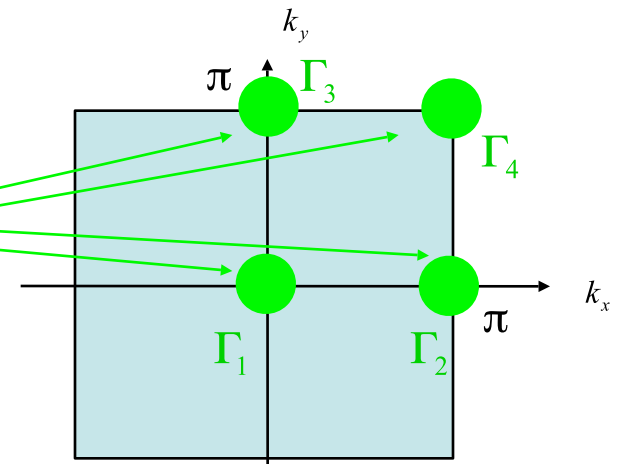


Z_2 topological number ν

$$(-1)^\nu = \prod_{i=1}^4 \prod_{m=1}^N \xi_{2m}(\Gamma_i)$$

± 1 : parity eigenvalue of the Kramers pairs at

$$\Gamma_i = \frac{\vec{G}}{2}$$



With inversion symmetry \rightarrow

-- product of parity eigenvalues over filled Kramers pairs over Γ_i

easy to calculate !

Candidate systems for quantum spin Hall phase?

- Nonmagnetic insulator
- Z_2 topological number = odd

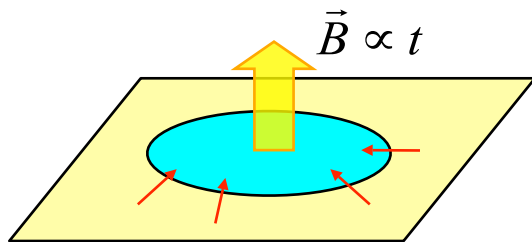
Spin Hall effect and Streda formula

Středa formula for Hall effect

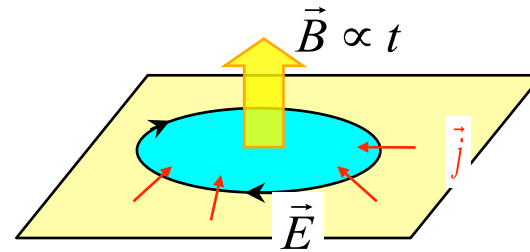
Středa (1982)

$$\sigma_{xy} = \sigma_{xy}^I + \sigma_{xy}^{II} \quad \left\{ \begin{array}{l} \sigma_{xy}^I = \frac{ie^2}{2} \text{Tr} \left[v_i \frac{1}{E_F - H + i0} v_j \delta(E_F - H) - \text{h.c.} \right] : \text{Fermi-energy term} \\ \sigma_{xy}^{II} = e \frac{dN}{dB} \Big|_{E_F} : \text{zero for insulator} \end{array} \right.$$

N : Number of states below E_F



$$\frac{dN}{dB} \Big|_{E_F} \text{ electrons flow in.}$$



$$j = E e \frac{dN}{dB} \Big|_{E_F} : \text{Hall current}$$

Charge \rightarrow spin

Středa formula for spin Hall effect

Expected result :

$$\sigma_s = \sigma_s^I + \sigma_s^{II}$$

σ_s^I : zero for insulator

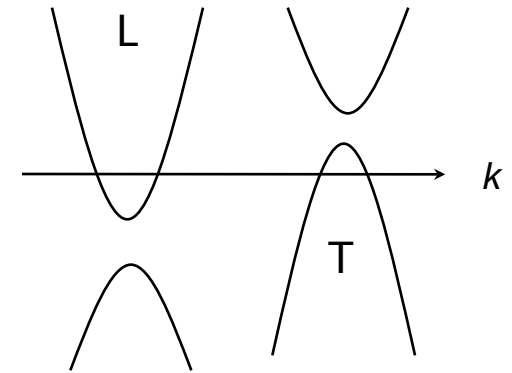
$$\sigma_s^{II} = \frac{dS_z}{dB} \Big|_{E_F}$$

: Spin-orbit susceptibility
 \leftarrow spin-orbit coupling

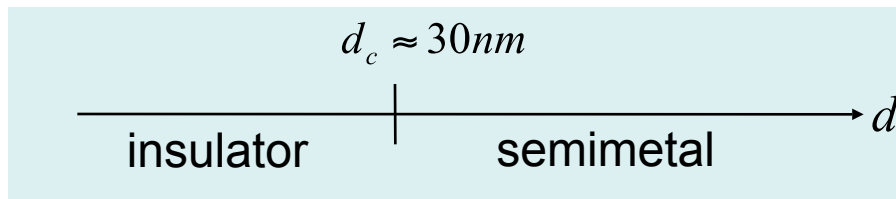
SM, PRL 97, 236805 (2006)

Candidate materials for QSH phase ?

- Bi – semimetal { hole pocket at T point
3 electron pockets at L points



Thin film – vertical motion quantized \rightarrow Gap opens



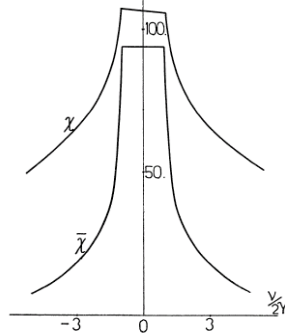
V. N. Lutskaa (1965)
V. B. Sandomirskii (1967)
C. A. Hoffman et al. (1993)

Enhanced diamagnetic susceptibility in Bi and $\text{Bi}_{1-x}\text{Sb}_x$

Interband matrix elements due to spin-orbit coupling

Theory

Fukuyama, Kubo (1970)



Experiment

Brandt, Semenov, Falkovsky (1977)

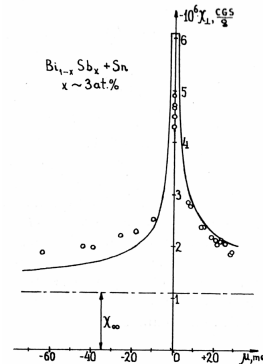


Fig. 6

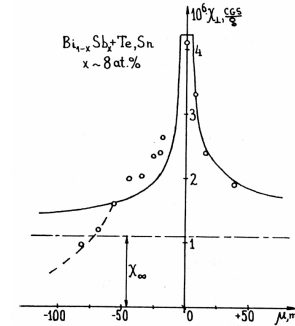
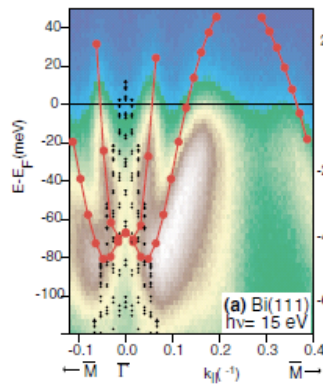


Fig. 7

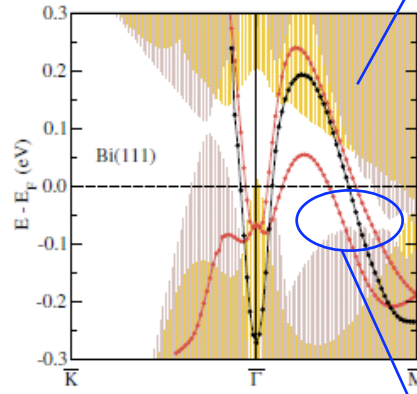
Surface states of Bi -- large spin splitting --

Large spin splitting in Bi (111)

Koroteev et al., PRL ('04).



(exp.)



(calc.)

bulk

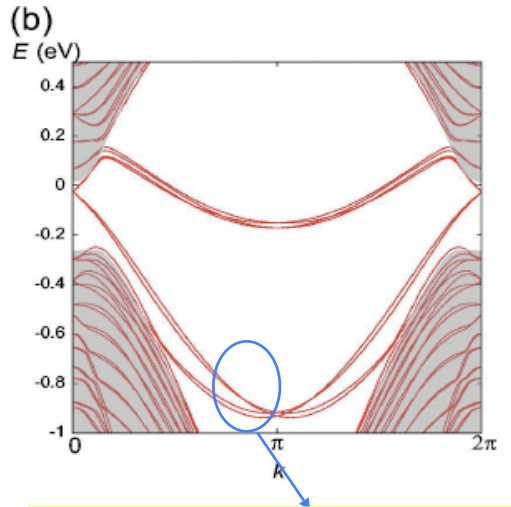
surface

- large spin splitting ($\approx 0.1\text{eV}$) = carry spin current
- surface states at E_F

2D bismuth as a candidate for QSH phase

SM
Phys. Rev. Lett.97, 236805(2006)

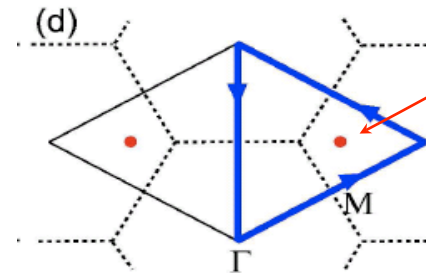
• Band structure for 2D strip



1 pair of edge states at each edge

• Z_2 topological number

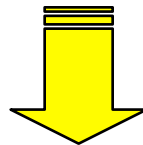
zeros of the Pfaffian in half Brillouin zone



$\nu = \text{odd}$

• spin Chern number

$$C_{sC} = -2$$



• Parity eigenvalues and Z_2 topological number

$$(-1)^\nu = \prod_{i=1}^4 \prod_{j=1}^N \xi_j(\Gamma_i)$$

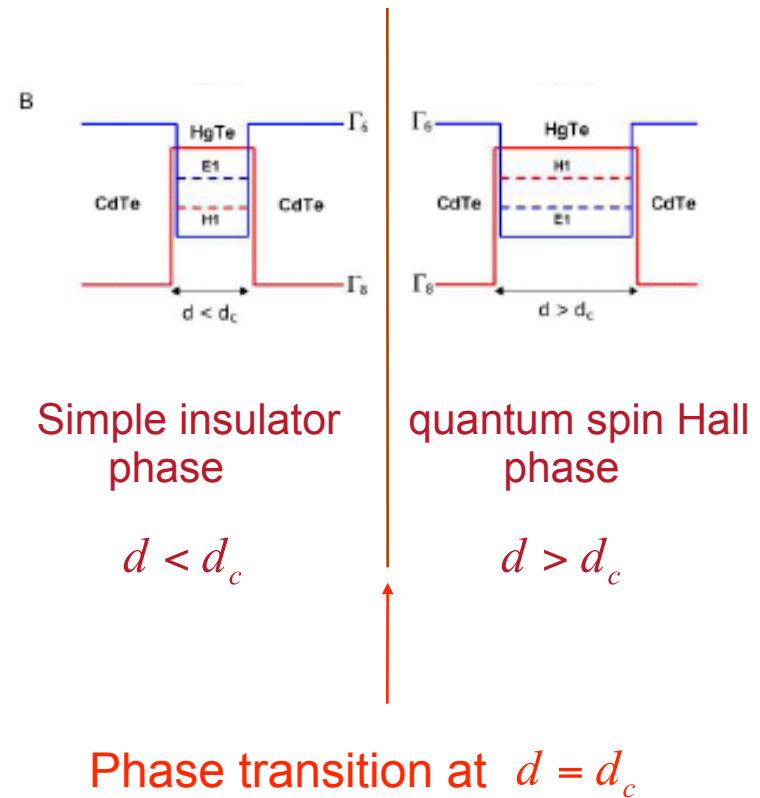
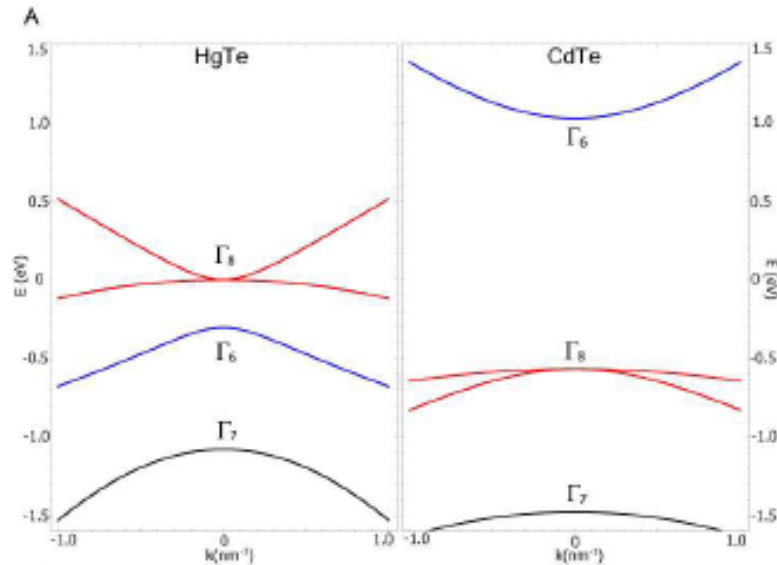
(← Fu, Kane cond-mat/0611341)

Conclusion

2D bismuth = good candidate for QSH phase !

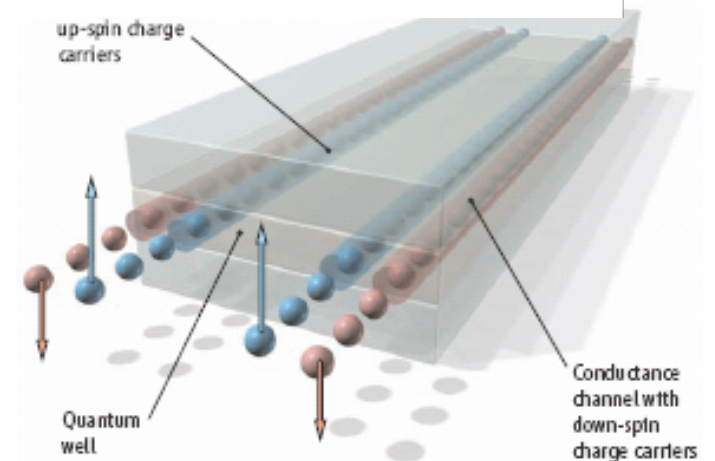
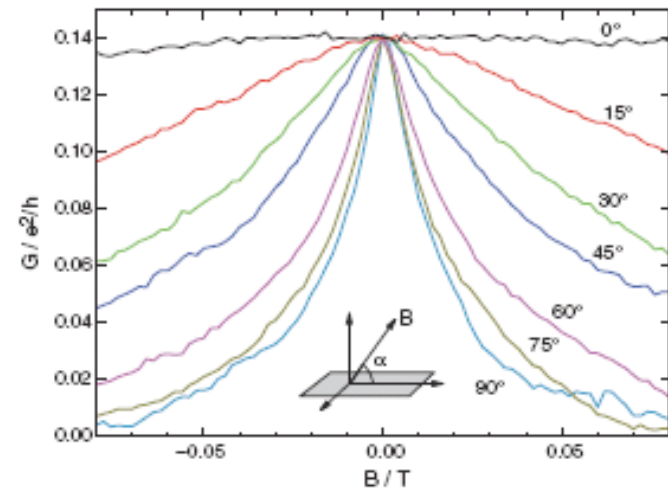
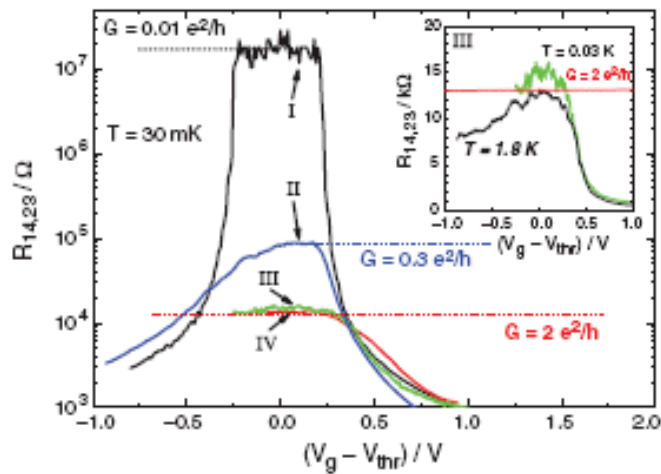
Other candidate systems : CdTe/HgTe/CdTe quantum well

M B. A. Bernevig, T. L. Hughes, S.-C. Zhang
Science **314**, 1757(2007);



Observation of QSH state in CdTe/HgTe/CdTe quantum well

Markus König, *et al.*
Science **318**, 766 (2007);



Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

3D quantum spin Hall phase

Z₂ topological number in 3D

- Only ν_0 is stable against disorder.

$\nu_0 = \text{even}$: weak topological insulator

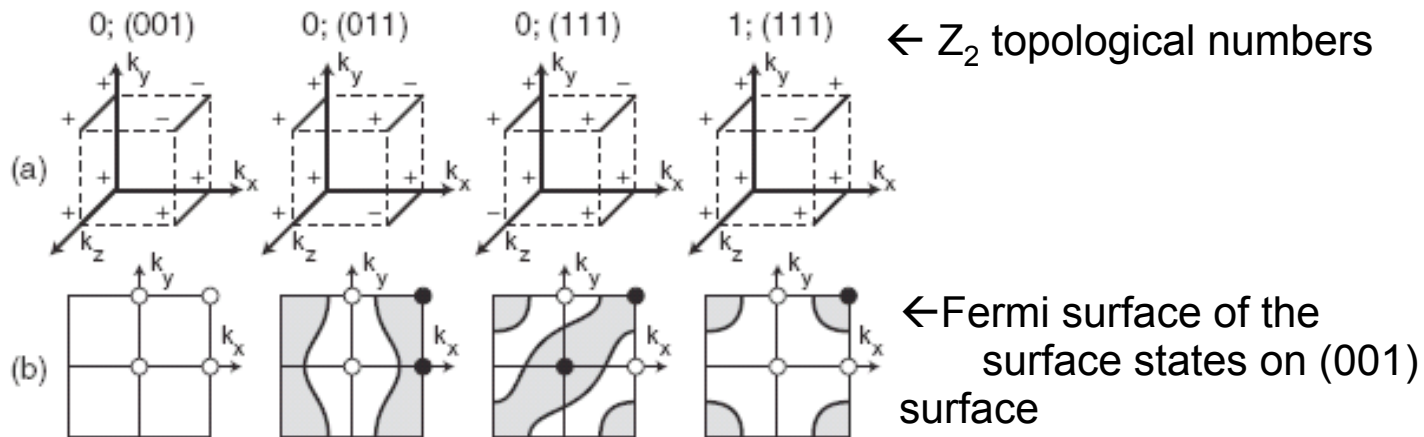
$\nu_0 = \text{odd}$: strong topological insulator
Topological surface states

$$(-1)^{\nu_0} = \prod_{\vec{k} \in \bar{G}/2} \delta_{\vec{k}}$$

$$\left(\begin{array}{l} \text{No inversion symmetry } \delta_i = \frac{\sqrt{\det[w(\Gamma_i)]}}{\text{Pf}[w(\Gamma_i)]} \\ \text{With inversion symmetry } \delta_i = \prod_{m=1}^N \xi_{2m}(\Gamma_i) \end{array} \right)$$

Materials for strong topological insulators (QSH phase) ?

Topology of the Fermi surfaces.



Candidate materials for 3D QSH phase

Fu, Kane, PRB(2007)

$\text{Bi}_{1-x}\text{Sb}_x$ ($0.07 < x < 0.22$)

α -Sn, HgTe under uniaxial pressure .

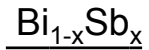
$\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ under uniaxial (111) strain

- Bi_2Te_3
- Kondo insulators
- skutterudites

(Thermoelectric materials ?)

Candidate materials for 3D QSH phase

Fu, Kane, PRB76, 045302 (2007)



Bi & Sb \rightarrow semimetal (direct gap >0 for every k)

Suppose the band overlap is lifted by perturbation
 = Z_2 topological number defined

Calculation of ν_0 from parity

Bismuth

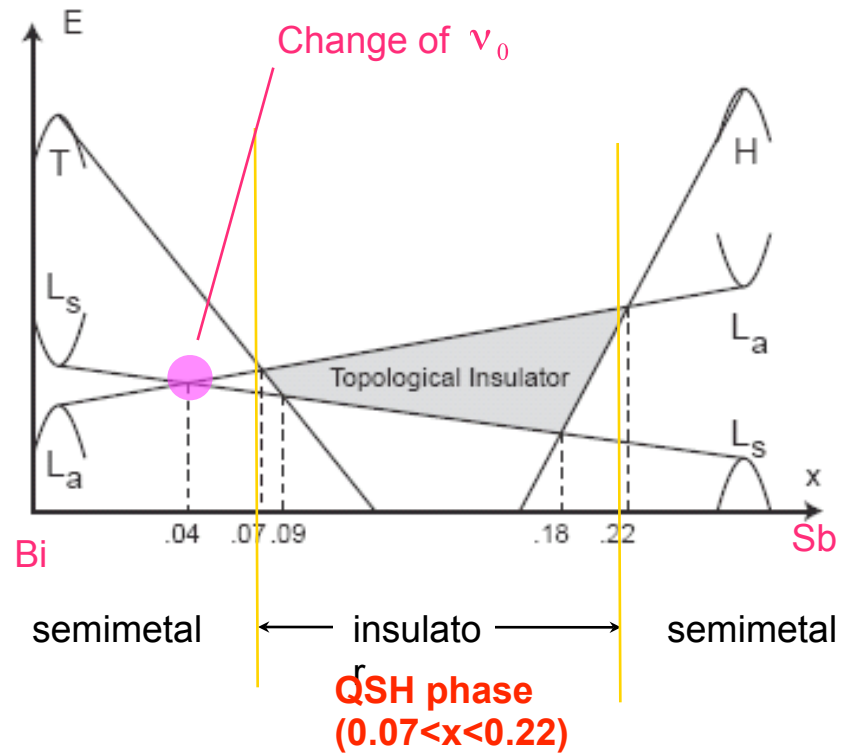
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	-
$3L$	L_s	L_a	L_s	L_a	L_a	-
$3X$	X_a	X_s	X_s	X_a	X_a	-
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	-
	Z_2 class					+

Even

Antimony

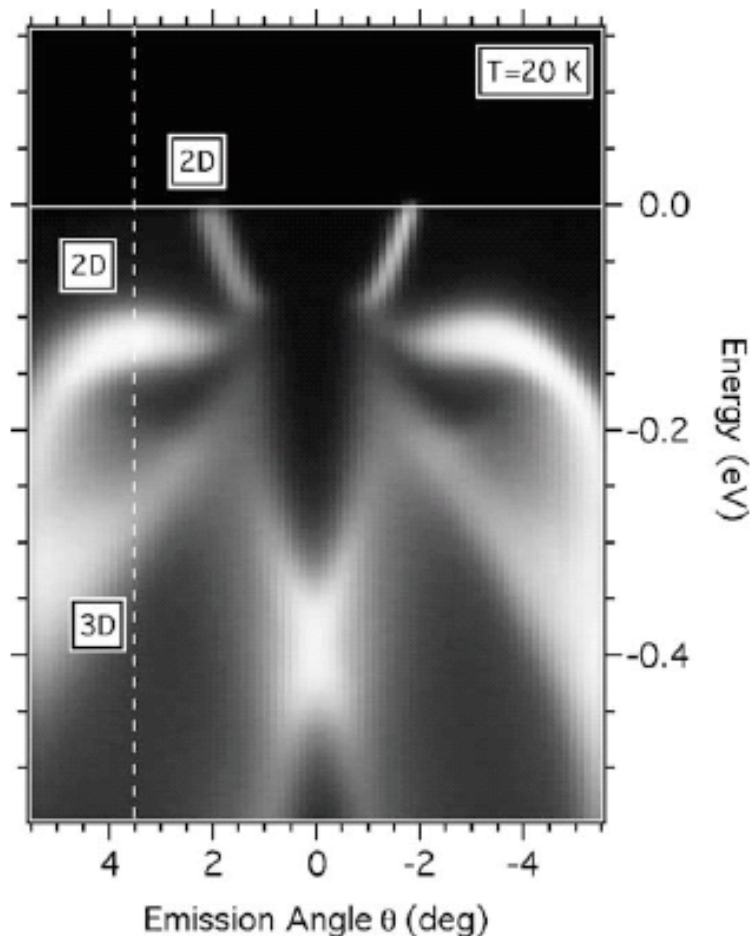
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	-
$3L$	L_s	L_a	L_s	L_a	L_s	+
$3X$	X_a	X_s	X_s	X_a	X_a	-
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	-
	Z_2 class					-

Odd
(but semimetal)

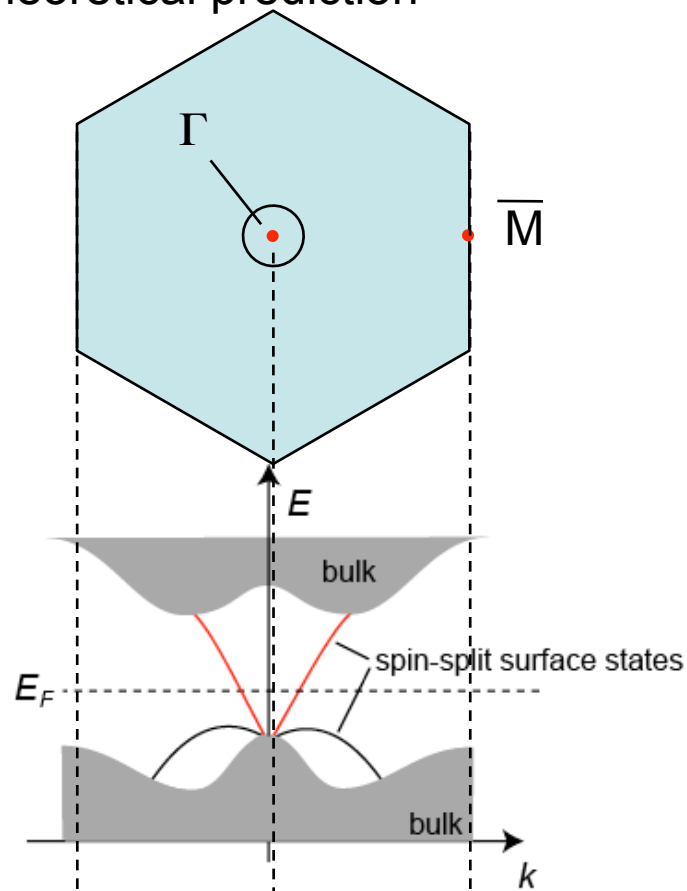


$\text{Bi}_{1-x}\text{Sb}_x$ ($0.07 < x < 0.22$) = QSH phase.

$\text{Bi}_{0.92}\text{Sb}_{0.08}$, (= theoretically in the QSH phase (Fu et al. (2006)))



Theoretical prediction

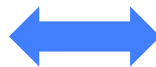


1 gapless fermion : Unique for a surface of 3D QSH system
cf. 2 gapless fermions in graphene (K and K' points)

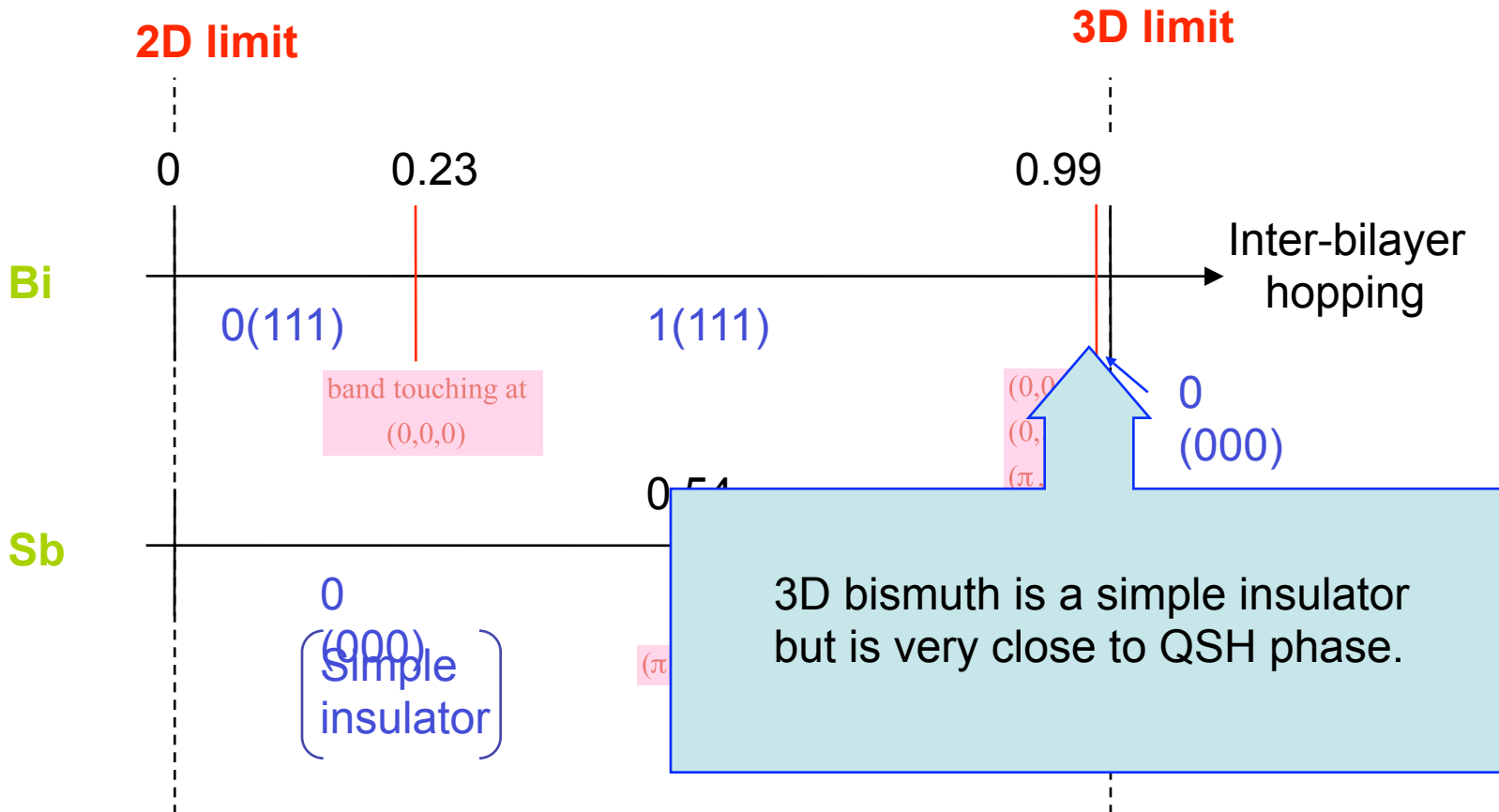
Phase transitions

See Fukui, Hatsugai, (2006)

- 2D : Bi: QSH
Sb: insulator
(Murakami, PRL (2006))

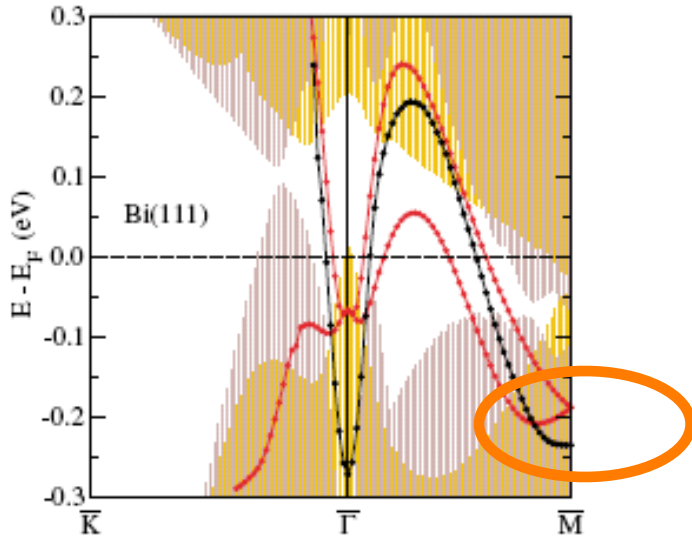


- 3D : Bi: insulator
Sb: QSH
(Fu,Kane,PRB(2007))

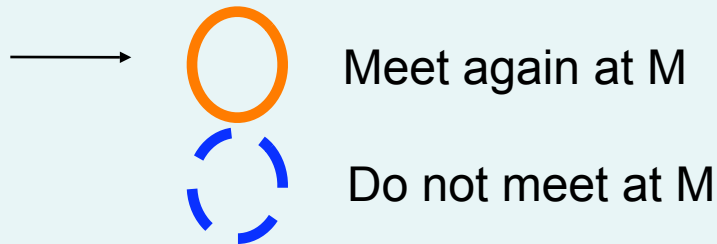


(111) surface

Koroteev et al., PRL (2004).

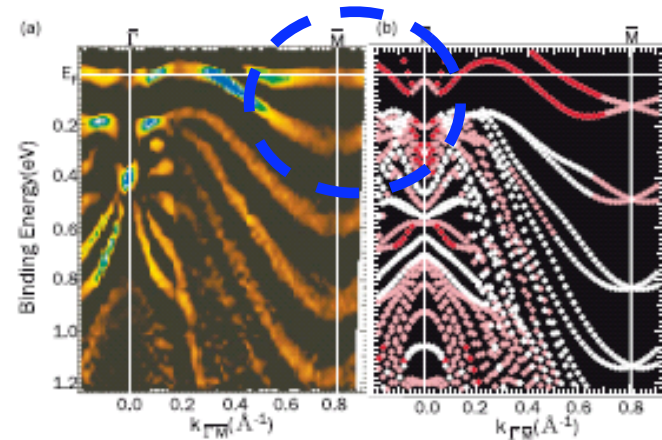


Rashba spin-split bands at Γ



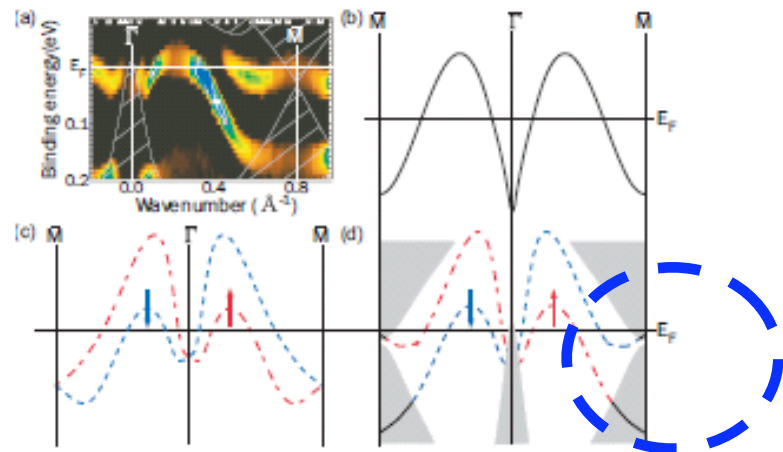
10-bilayer (111)-bismuth

Hirahara et al., PRL (2006)



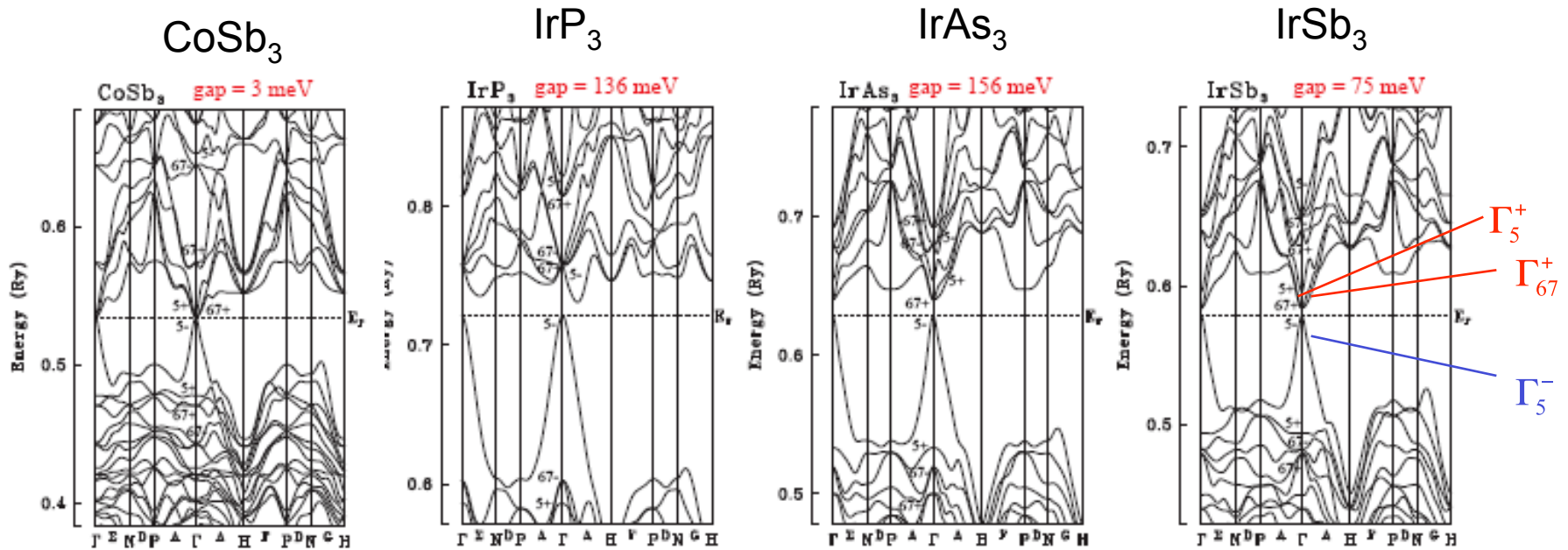
Hirahara et al., preprint (2007)

Spin-resolved ARPES



Rashba spin splitting

(Example) binary skutterudite (Thanks to K.Takegahara (Hirosaki))



$$\vec{k} = \vec{\Gamma}_i = \frac{1}{2} (n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3) \quad (n_i = 0, 1) \longrightarrow \Gamma, H, N \times 6$$

Z_2 topological number ν

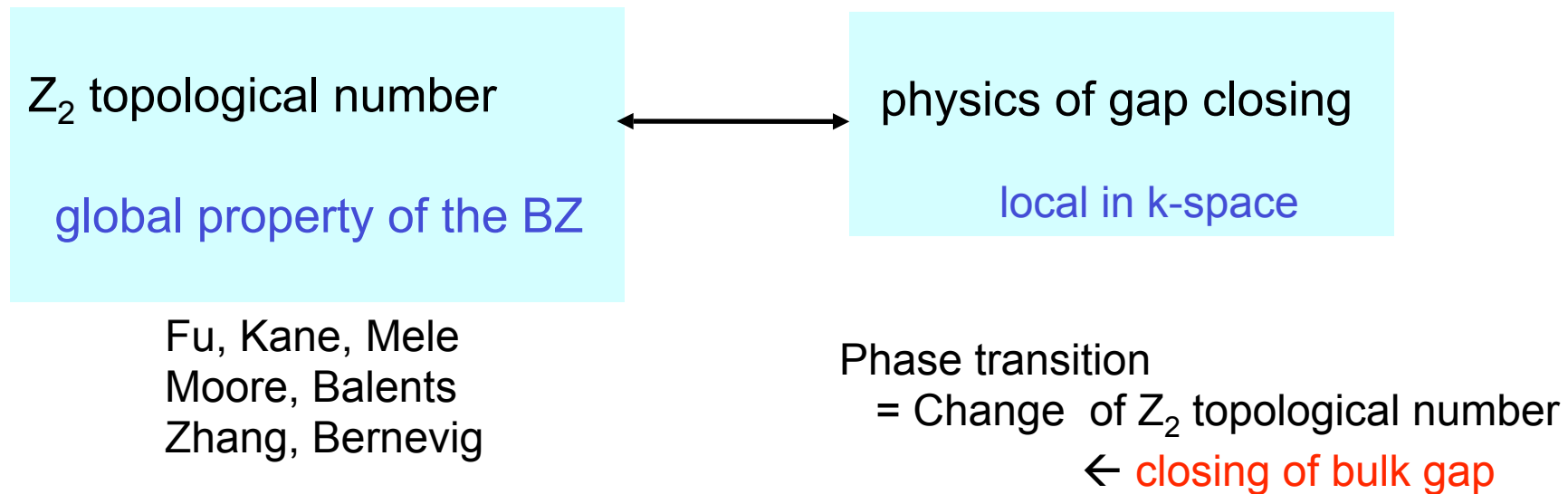
$$(-1)^\nu = \prod_{\Gamma, H, 6N} \prod_{m=1}^N \xi_{2m}(\Gamma_i) = +1 \quad : \text{Ordinary insulator}$$

Parity (= ± 1)

Phase transition

between the quantum spin Hall and insulator phases

- How does the gap close?

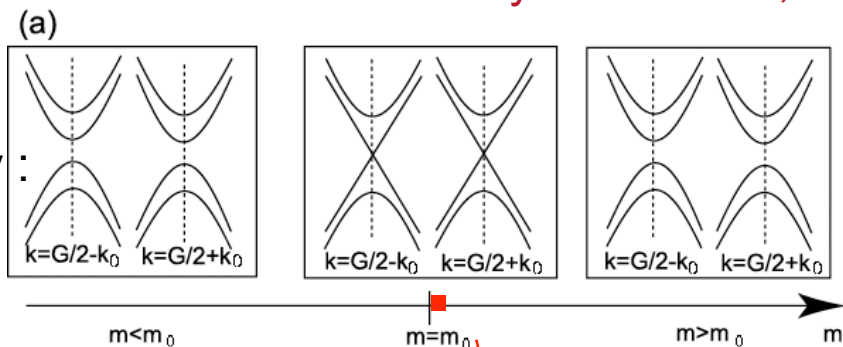


Phase transition between QSH and insulator phases

2D

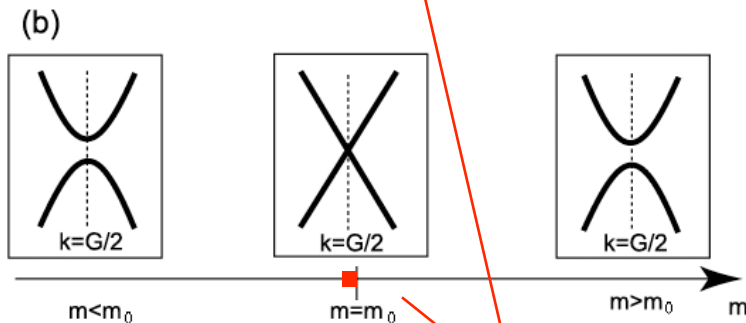
(SM, Iso, Avishai, Onoda, Nagaosa, Phys. Rev. B76, 205304 (2007))

• No inversion-symmetry :



Honeycomb lattice model
Kane, Mele,
PRL (2005)

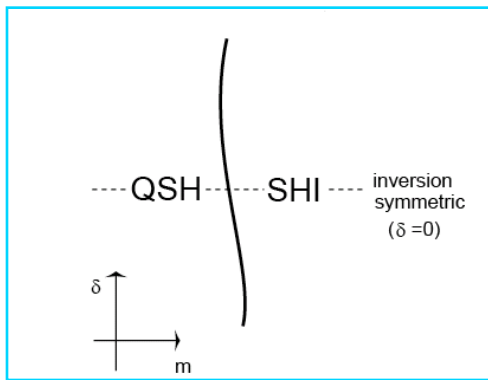
• Inversion-symmetry :



CdTe/HgTe/CdTe QW
Bernevig et al.,
Science (2006)

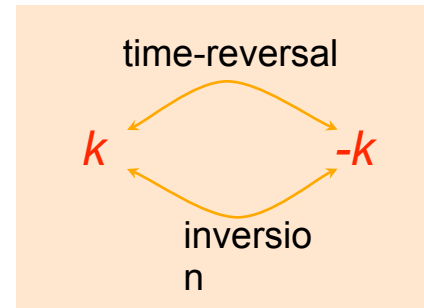
transition

Phase diagram



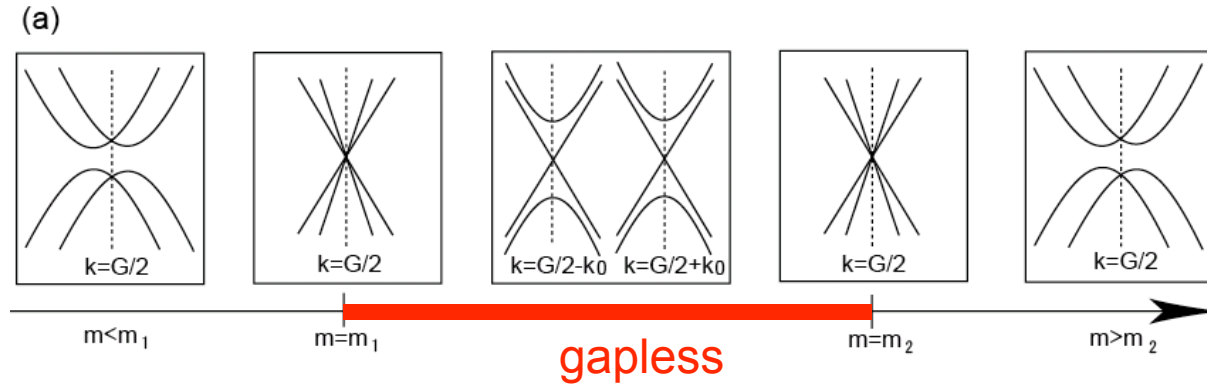
Phase transition between QSH and insulator phases

(SM, New J. Phys. (2007))

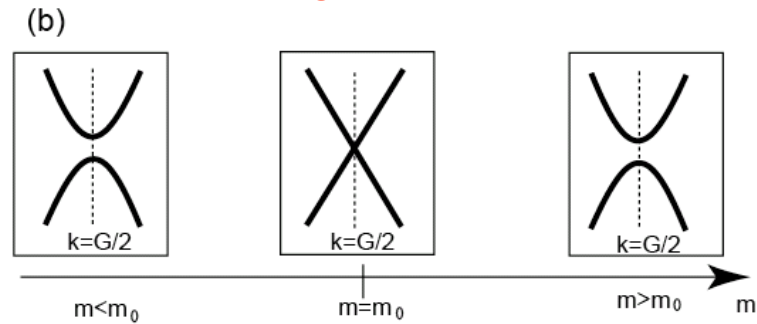


3D

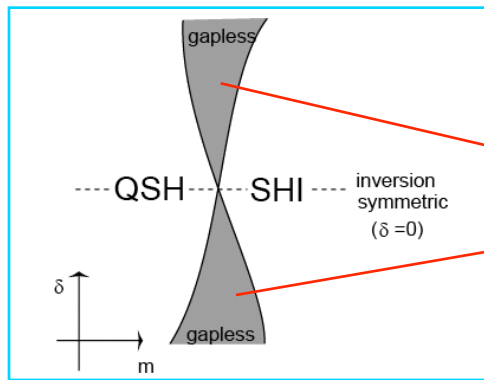
• No inversion-symmetry :



• Inversion-symmetry :



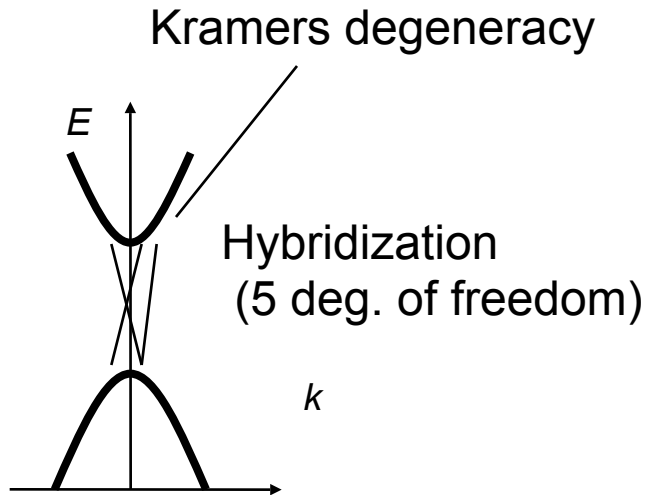
Phase diagram



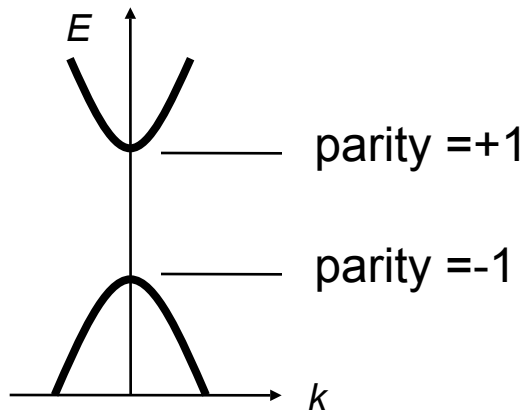
Topological gapless phase

Phase transition between QSH and insulator phases

inversion-symmetric



One-parameter tuning
→ no gap closing

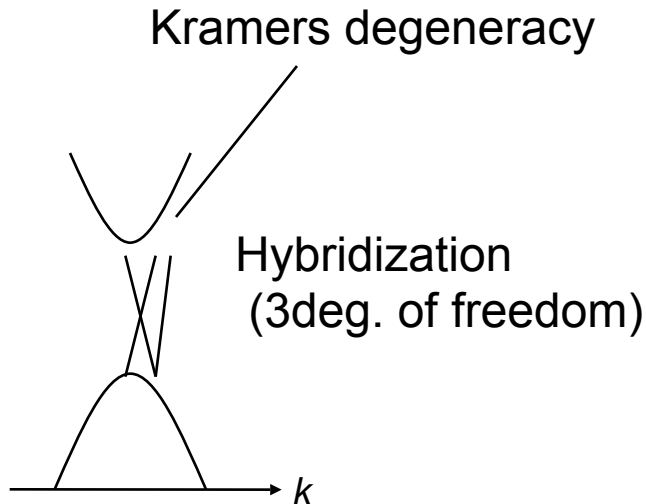


Some hybridization matrix elements vanish.

Can close the gap
by one-parameter tuning

Phase transition between QSH and insulator phases

No inversion-symmetric



- 2D : 3 variables

$$\vec{k} = (k_x, k_y), m$$

Can close the gap
by one-parameter tuning

- 3D : 4 variables

$$\vec{k} = (k_x, k_y, k_z), m$$

One extra parameter
→ Gap closing = a curve in the hyperspace

$$(k_x, k_y, k_z, m)$$

3D systems **without** inversion-symmetry

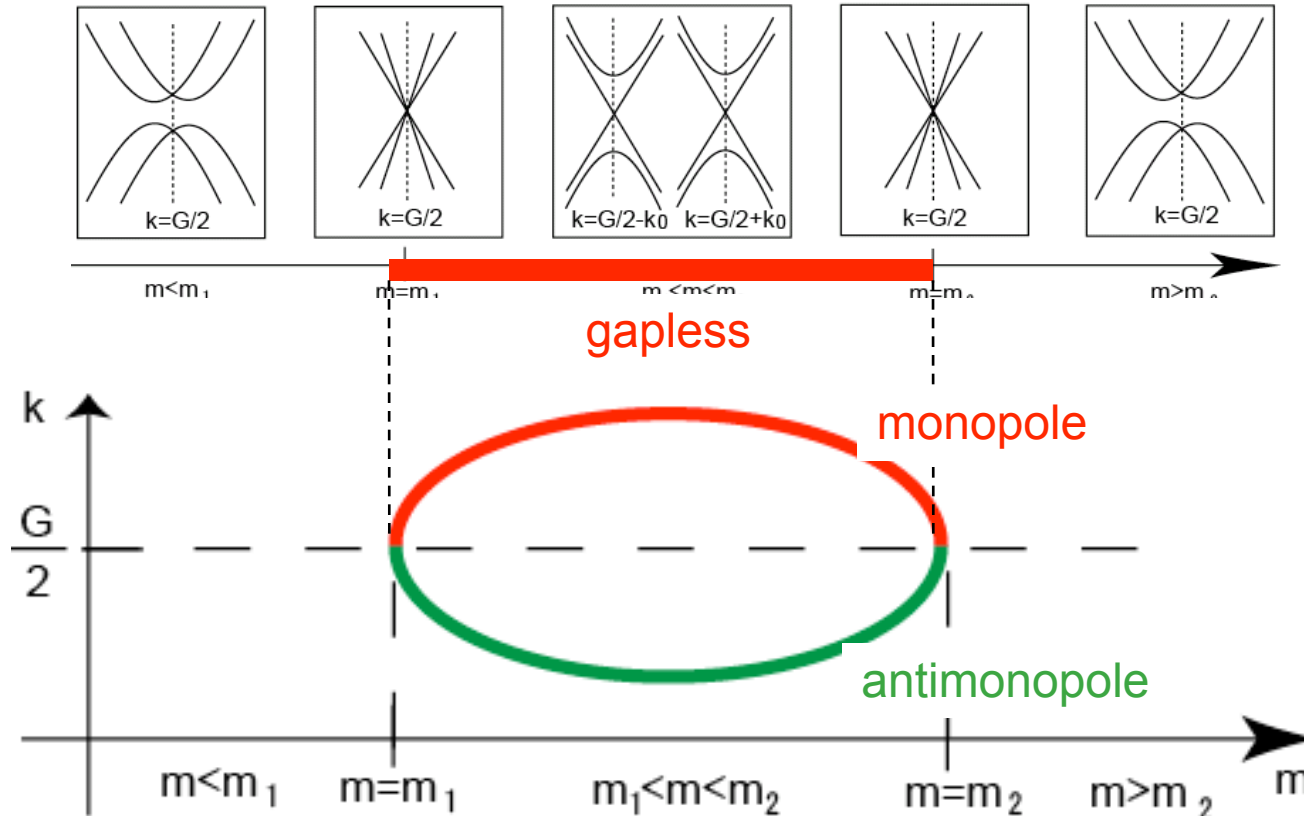
(SM, New J. Phys. (2007))

Phase transition at $m = m_0$: impossible

Instead, gapless phase appears between QSH and insulator phases.

$$m_1 \leq m \leq m_2$$

Pair creation of monopole and antimonopole in k-space



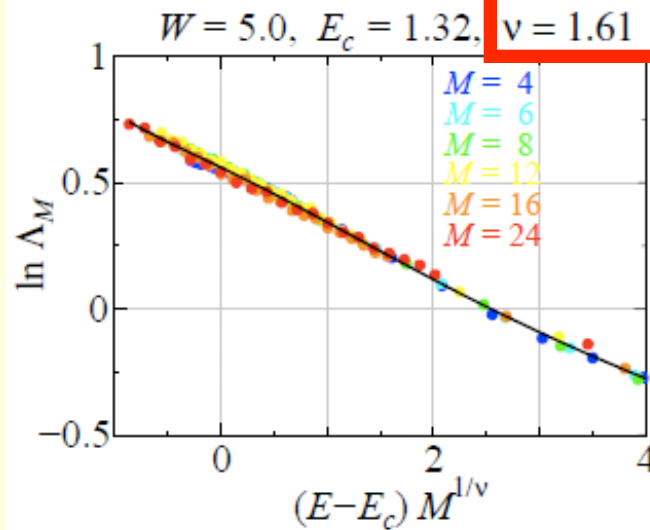
Universality classes of Anderson Localization

Time-reversal symmetric system
with the **spin-orbit interaction**
(**symplectic** universality class)

Scaling Analysis for QSH phase

Onoda, Avishai, Nagaosa, cond-mat/0605510

$$\xi \approx (E - E_c)^{-\nu}$$



Different from

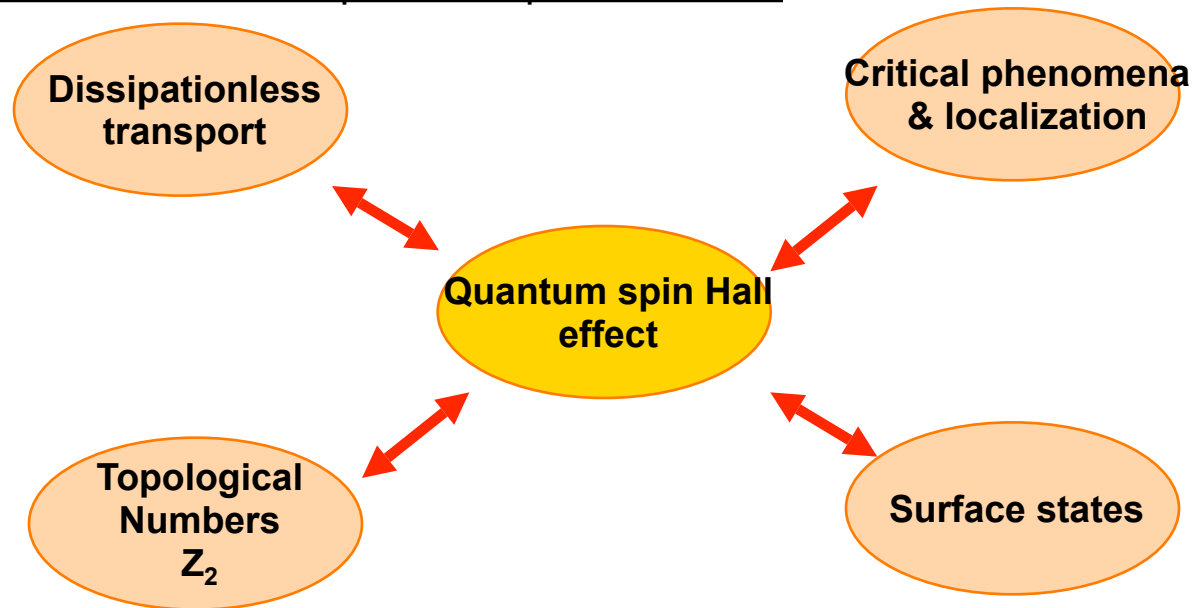
$$\nu_{\text{symplectic}} = 2.73$$

$$\nu_{\text{unitary}} = 2.33$$

New universality class?

Why is the quantum spin Hall effect interesting?

- Various fields are related with quantum spin Hall effect



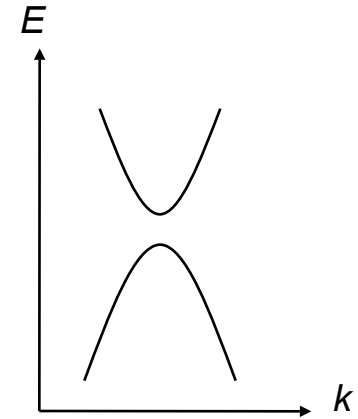
- topological order in nonmagnetic insulators
- perfectly conducting channel
- No magnetic field required
(cf. quantum Hall effect – requires strong magnetic field)
- Only 1 gapless fermion: **Unique for a surface of 3D QSH system**

(cf. In 2D systems, number of fermions is even (fermion doubling)
2 gapless fermions in graphene)

Summary

Spin Hall effect in metals and semiconductors

- p-type \gg n-type
- Enhanced at band crossing
Pt : large spin Hall effect



Quantum spin Hall effect:

- 2D & 3D
- Edge states
--- topologically protected
- Bismuth and surface states \rightarrow spin current
- Phase transition between the quantum spin Hall phase and ordinary insulator phase.

Topological gapless phase in 3D

