Topological Physics in Band Insulators III

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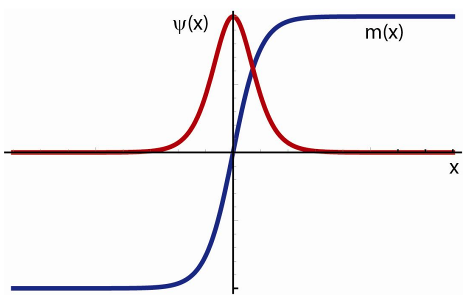
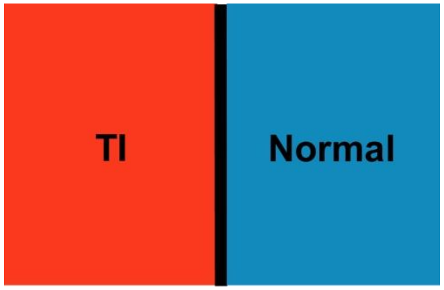
Low energy models for real materials

Summary of Second Lecture: A two-valued integer index distinguishes conventional and topological insulators. A change of this index at a boundary between insulators signals the existence of symmetry-protected Dirac modes propagating along the interface.





Summary of Third Lecture: This physics is realized in a family of 2D and 3D crystalline solids. **Goal**: connect band theoretic analysis of the bulk and low energy representation of its protected interface states.

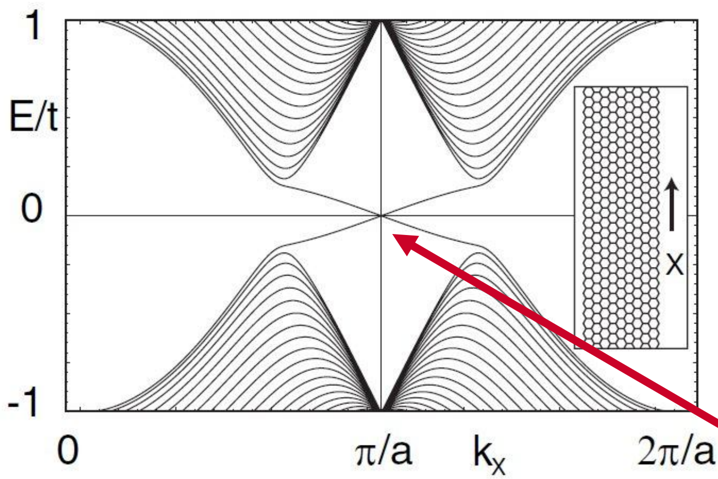
Gapping the Graphene Dirac Point

$\sigma_x \tau_x, \sigma_x \tau_y$	Kekule: valley mixing	spinless
σ_z	Heteropolar (breaks P)	spinless
$\sigma_z \tau_z$	Modulated flux (breaks T)	spinless
$\sigma_x \tau_z s_y - \sigma_y s_x$	Spin orbit (Rashba, broken z→-z)	
$\sigma_z \tau_z s_z$	Spin orbit (parallel)*	

*This term respects all symmetries and is therefore present, though possibly weak

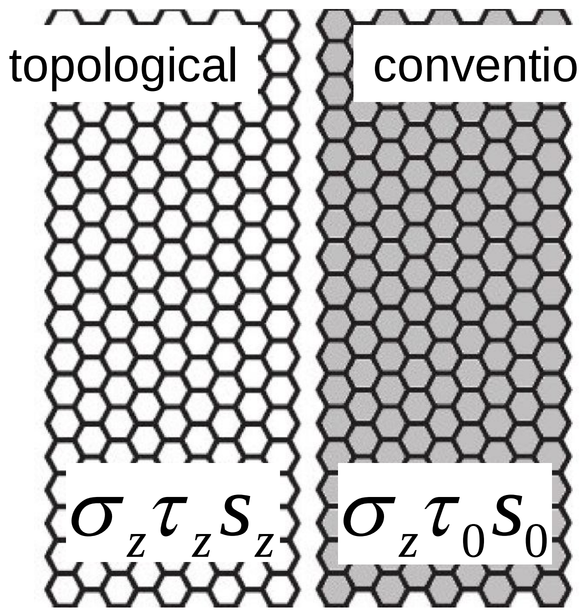
For carbon **definitely** weak

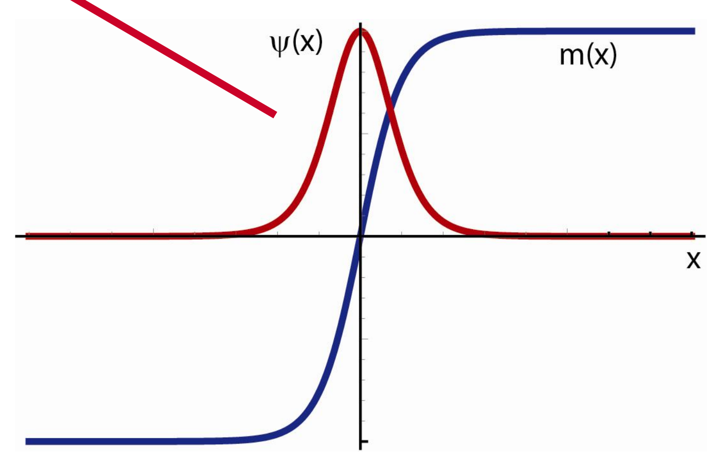
Spin-filtered edge states



Counterpropagating spin-filtered edge states

Edge: Hamiltonian undergoes a **single** mass inversion (at K or K') in each spin sector





Comments

The energy scale for this effect is very small (carbon is a light atom)

But the physics is robust (topological)

Hybrid structures:
"enhance" spin orbit field from adsorbed heavy metallic species

Spin-orbit coupled semiconductors:
Band inversion occurs in narrow gap semiconductors with strong s-o coupling

History: special interface states at a band-inverting junction

B. A. Volkov and O. A. Pankratov, JETP Lett. 42, 178 (1985)

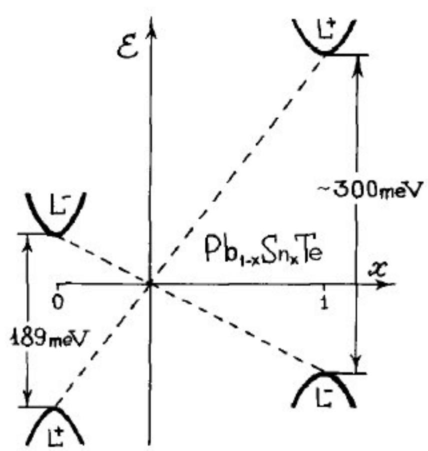


Fig. 1. The $Pb_{1-x}Sn_xTe$ band diagram. The degree non-symmetry of the diagram (the shift of a middle energy) is not established definitely.

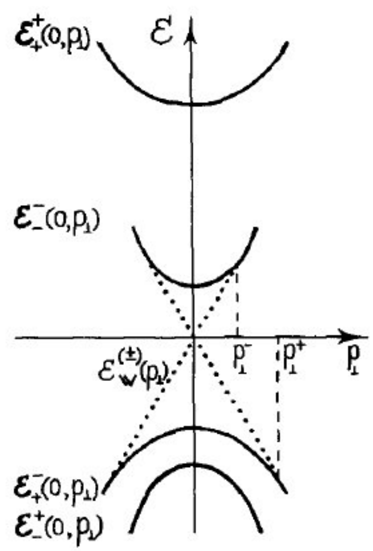


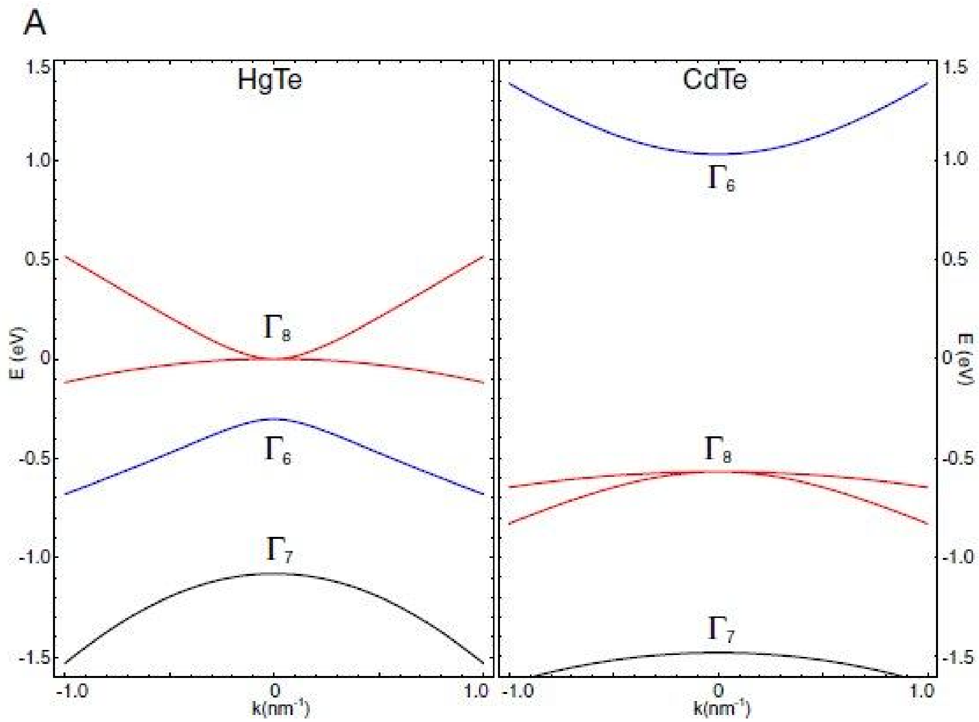
Fig. 3. Weyl spectrum (dotted lines) in a $Pb_{1-x}Sn_xTe$ band-inverting contact. The bands $\epsilon_-^{\pm}(0, p_\perp)$ to the left and $\epsilon_+^{\mp}(0, p_\perp)$ to the right of a contact, correspond to $L\pm$ terms and are taken at $p_z = 0$.

$Pb_{1-x}Sn_xTe$ alloys: interface states controlled by asymptotics

Band inversion in II-VI semiconductors

J=3/2
bonding p

J=1/2
antibonding s



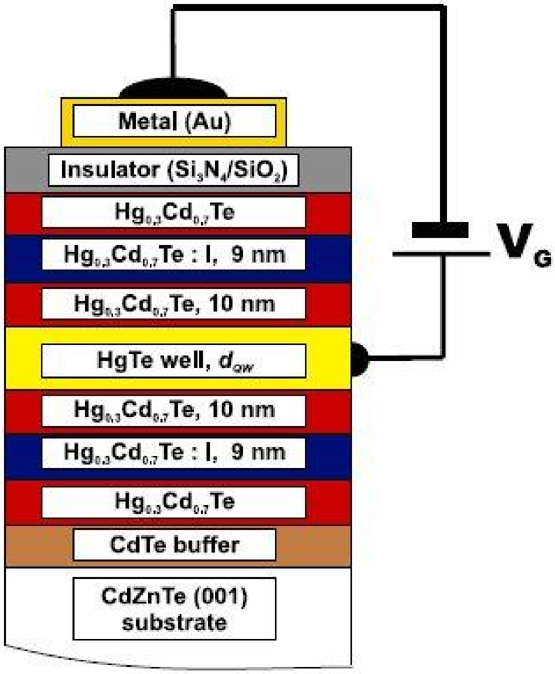
J=1/2
antibonding s

J=3/2
bonding p

“inverted”

“conventional”

Recent history: level ordering in a II-VI (001) quantum well



k=0 states are indexed by **axial symmetry**

$$\Psi_{\pm 1/2} = \alpha \left| \Gamma_6, \pm 1/2 \right\rangle + \beta \left| \Gamma_8, \pm 1/2 \right\rangle$$

$$\Psi_{\pm 3/2} = \left| \Gamma_8, \pm 3/2 \right\rangle$$

With low energy space spanned by 4x4

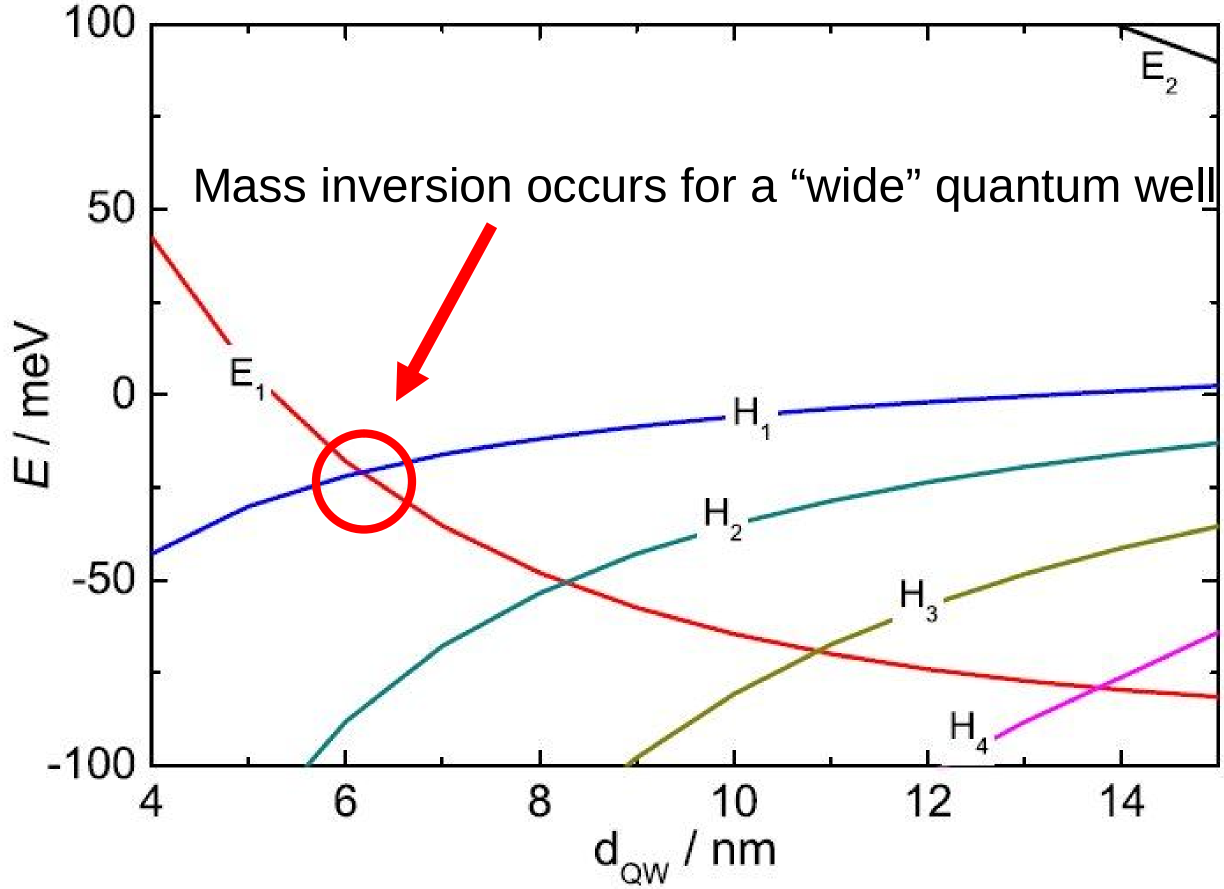
$$H(k_x, k_y) = \begin{pmatrix} h(k_x, k_y) & 0 \\ 0 & h^*(k_x, k_y) \end{pmatrix}$$

“Decoupled 2x2 blocks”

Konig et al (Molenkamp group) (2007)

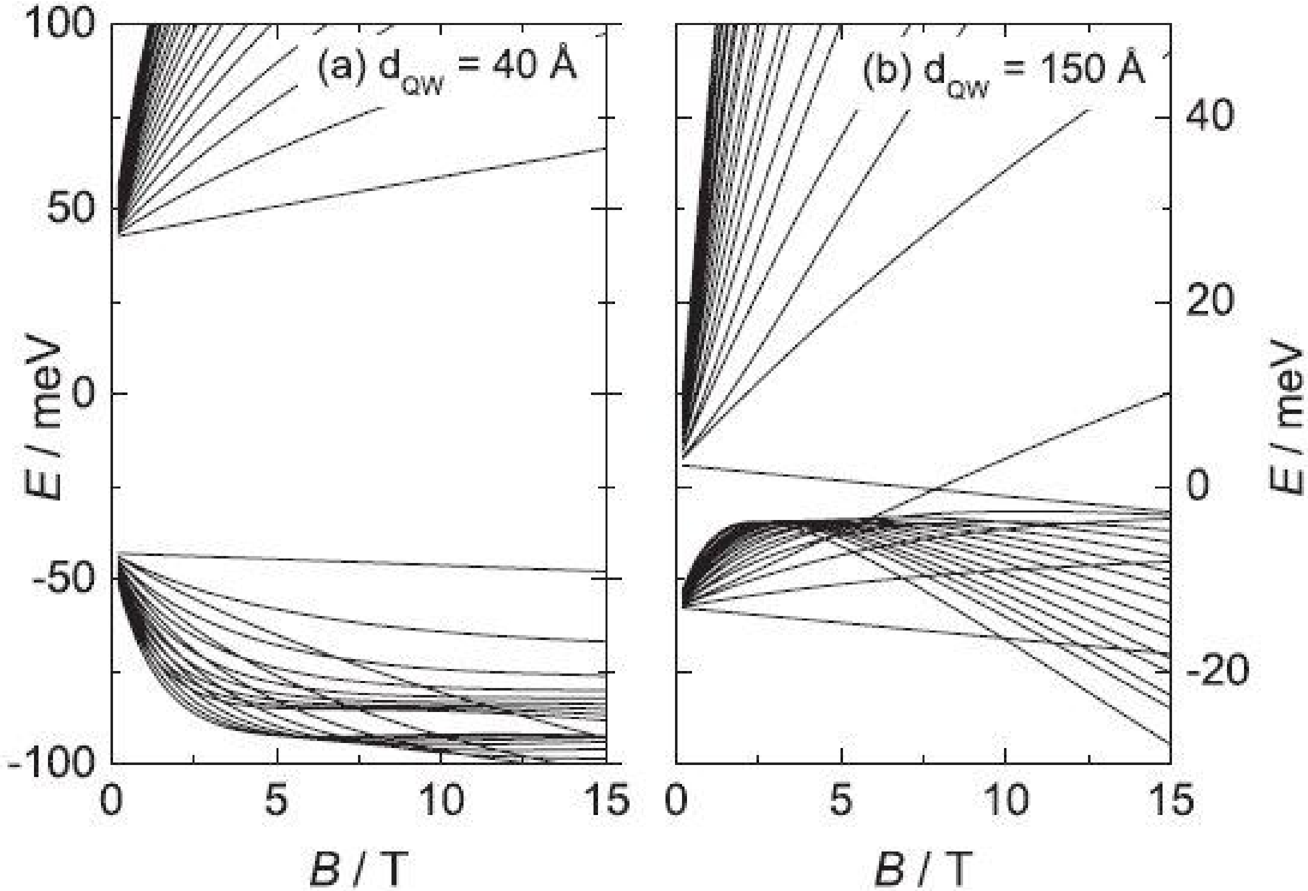
Representation as two state system

$$h(k_x, k_y) = \varepsilon(k)\mathrm{I}_{2\times 2} + \vec{d}(\vec{k}) \cdot \vec{\sigma}$$



Bernevig, Hughes and Zhang (BHZ, 2006)

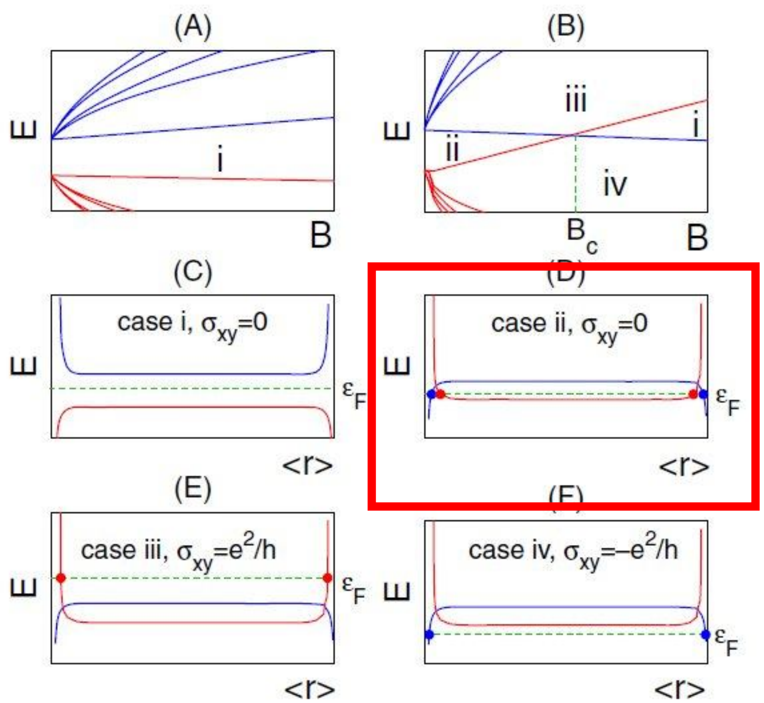
with anomalous Landau quantization

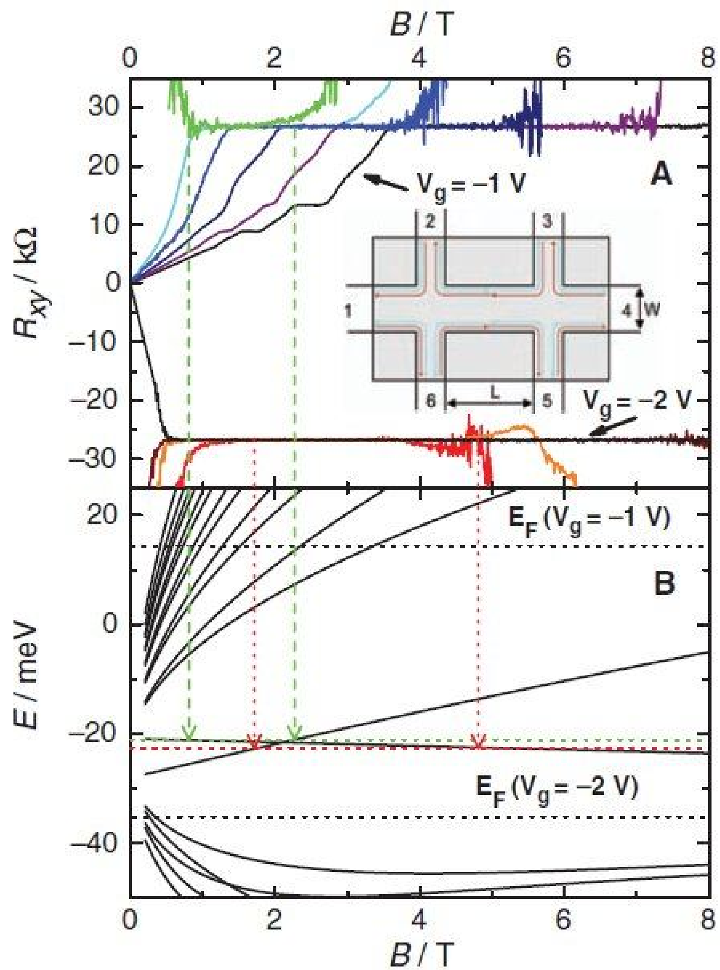


conventional

inverted

2D QSHE is observed via ballistic transport through its edge modes





Molenkamp group (2007, 2008)

2D experimental status

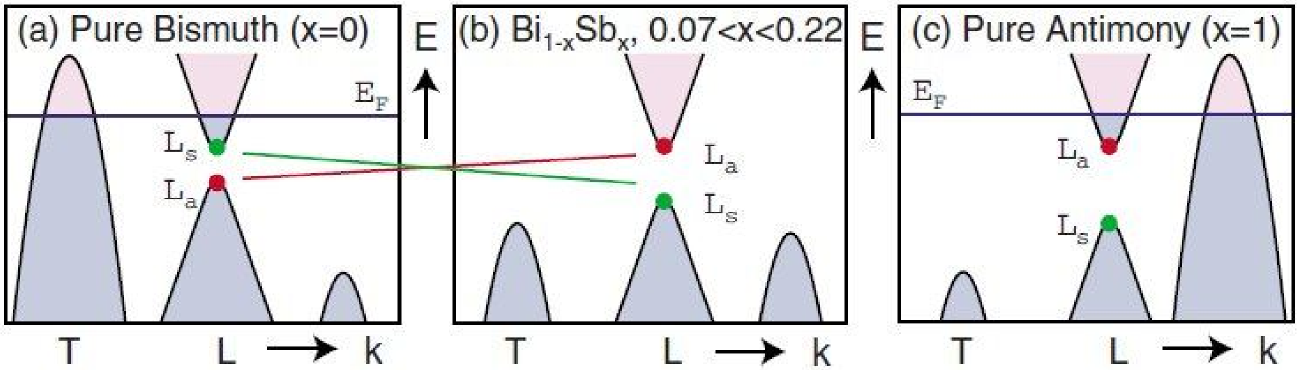
The realization of 2D QSHE in HgTe quantum wells requires strong spin-orbit coupling and broken cubic symmetry in a thin heterostructure.
(challenging fabrication, T~30 mK, B~ 10 T)

The "decorated graphene" strategy remains an unsolved experimental challenge.

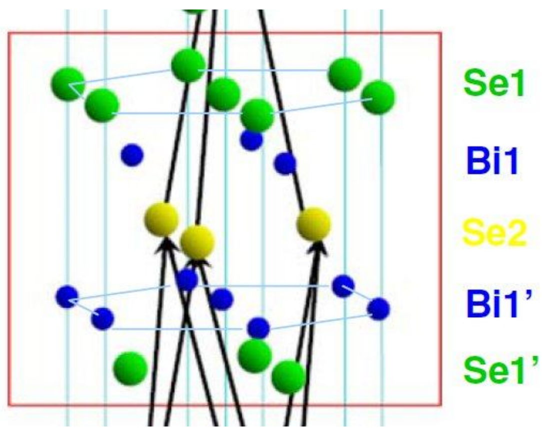
Amazingly, this physics occurs spontaneously in 3D materials that are readily synthesized and measurable at RT.

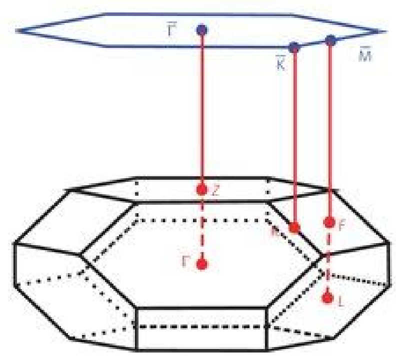
Examples in 3D

Alloys of Bi_xSb_{1-x} : Band inversion at three L points. Z_2=-1 for range of x



Bi_2Se_3 and related tri-chalcogenides. Stacked quintuple layers.

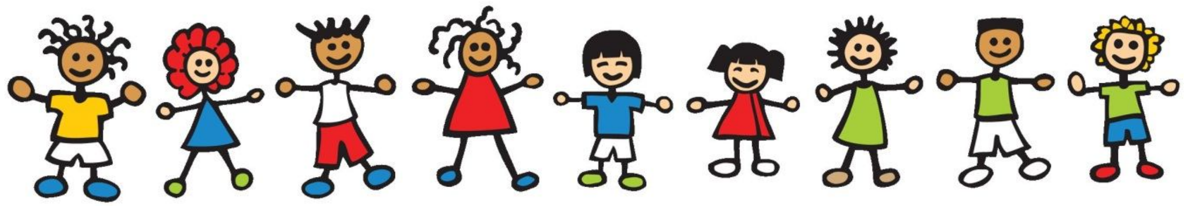




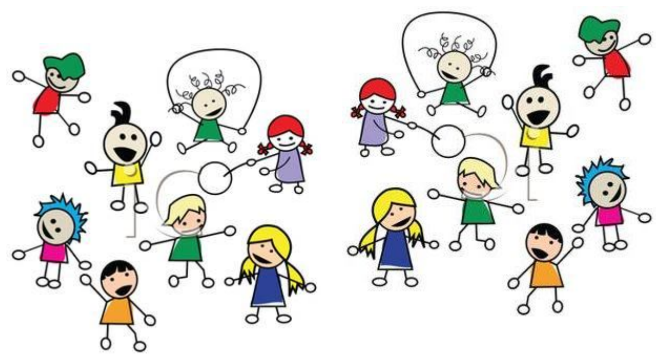
Mass reversal → interface state → spin texture

A kindergarten metaphor

1D Edge of a 2D Topological Insulator is like this



2D Boundary of a 3D Topological Insulator is more like

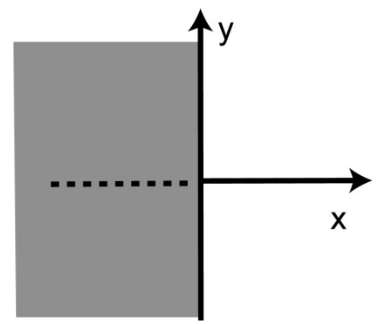


P.G. Silvestrov, P.W. Brouwer and E.G. Mischenko "On the structure of surface states of topological insulators" arXiv:1111.3650v3
A. Medhi and V.B. Shenoy "Continuum Theory of Edge States of Topological Insulators" arXiv:1202.3863v1
F. Zhang, C.L. Kane and GM "Surface States of Topological Insulators" arXiv:1203.6382v1

2D topological insulators admits a simple theory of the 1D helical edge states

S.C. Zhang group (2009)

Outline of calculation in 2D :



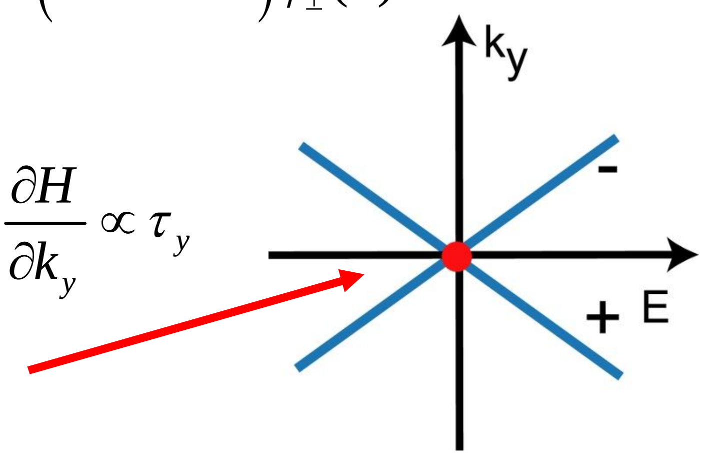
1. linearize 4 band $\tau \otimes \sigma$ model:

$$H(k_y) = H(k_y = 0) + \frac{\partial H}{\partial k_y} k_y + \dots$$

2. $H(k_y = 0)$ with node at x=0 admits Kramers degenerate evanescent solutions: $\psi_{\pm}(x) = a\left(e^{\lambda_1 x} - e^{\lambda_2 x}\right)\phi_{\pm}(x)$

with $\tau_y \phi_{\pm}(x) = \pm\phi_{\pm}(x)$

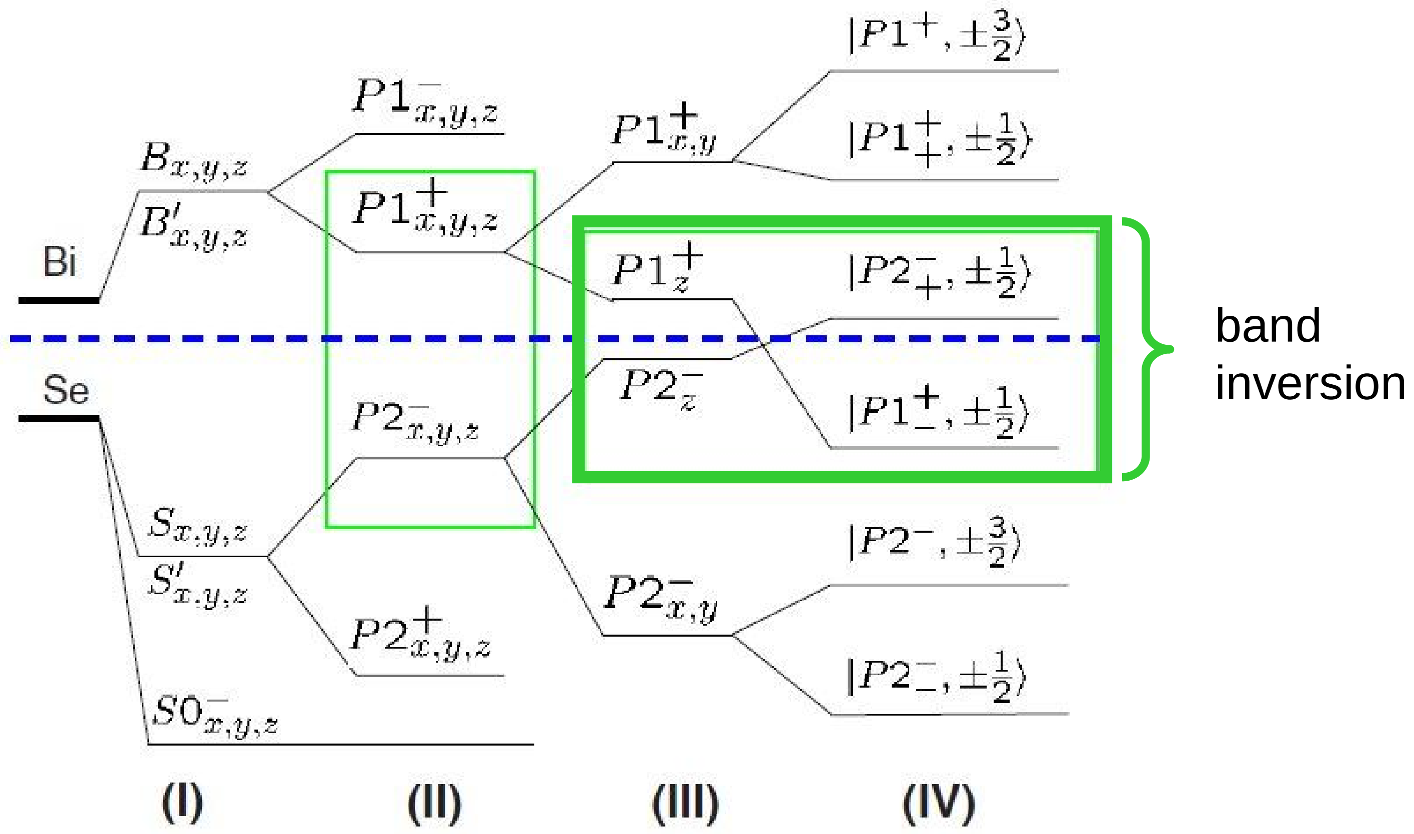
3. Bulk model prescribes $v_y = \dfrac{\partial H}{\partial k_y} \propto \tau_y$



the protected edge state is robust
but this result is fragile

Level ordering in Bi_2Se_3

Layered structure $R\bar{3}m$



atoms bonds parity crystal field spin orbit

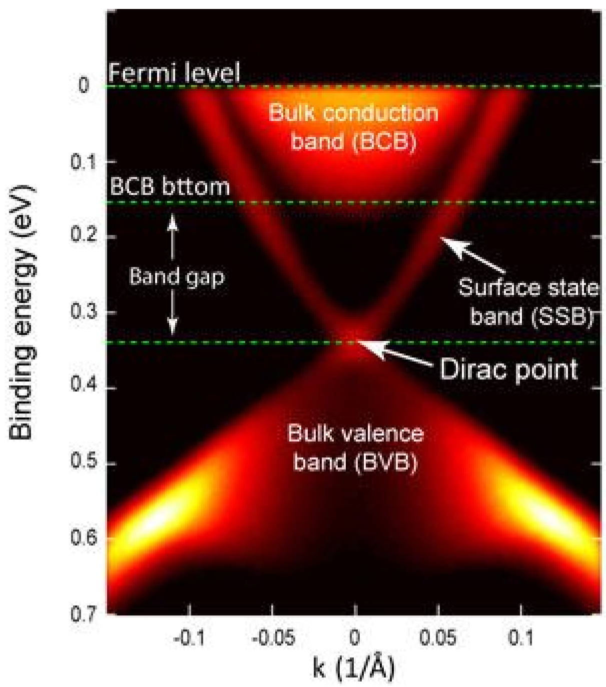
H. Zhang et al (Shoucheng Zhang group, 2009)

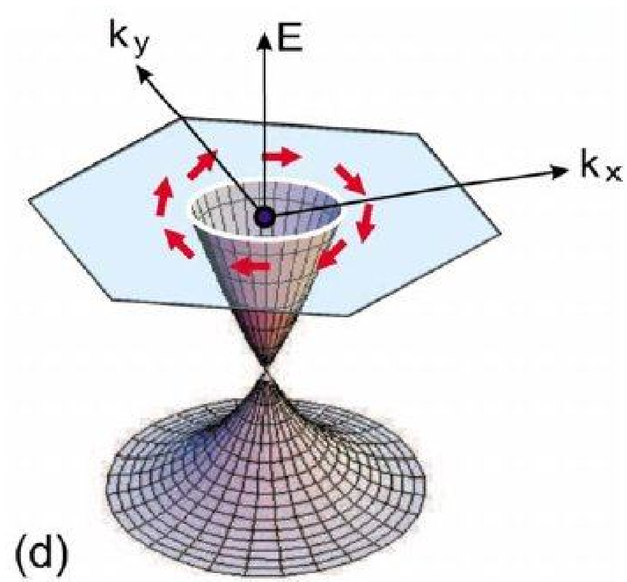
Bi_2Se_3 as TI Prototype

Eight bulk time reversal invariant momenta: Γ, Z, F(3), L(3).

Band inversion is **confined to small momenta** near Γ (occupied bands "buried" at seven other TRIM).

Hasan/Cava (2009)





ARPES: Single symmetry-protected Dirac cone measured on the (001) face

Graphene	Topological Insulator
Pairs of DP's (chiral partners)	Single DP (partner on opposite face)
Gapped by T-preserving σ_z potential (breaks P)	Ungapped by any T-preserving (protected Kramers pair)
Spin and valley degeneracies hide odd half-integral QHE	Odd half-integral QHE on a single face (TI=1/4 graphene)
$h = v\vec{\sigma}\cdot\vec{p}$ (helical)	$h = v\,\hat{n}\cdot\vec{\sigma}\times\vec{p}$ (twisted, chiral)
N/A	Face-dependent spectra: topological continuity via side faces
Weak trigonal warping	Strong hexagonal warping
g ~ 2	g ~ 30
Small quantum corrections in MR	Weak antilocalization in both surface and bulk channels

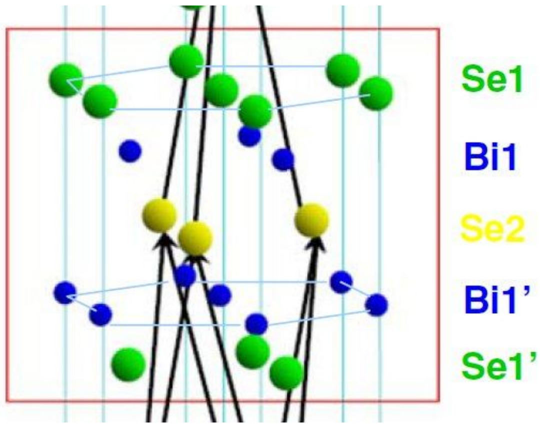
Topological Insulator Surface States

Bulk Boundary Correspondence:
The properties of the edge modes are determined by the bulk symmetries of the materials joined at the interface. (i.e. mass reversal)

Single Valley Physics:
Bi_2Se_3 –type materials have a **single** band inversion near Γ. The long wavelength theory is a gradient expansion within a single valley (minimal model).

Bulk Anisotropy:
The bulk Hamiltonian is **not isotropic** (Bi_2Se_3 is a layered material). Surface properties are therefore strongly face-dependent.

Bulk Hamiltonian



Four band model

(Bi(p_z^+), Se(p_z^-), $J_z=\pm 1/2$): $\tau \otimes \sigma$

Symmetries:

$C_2(x),\ C_3(z),\ P=\tau_z, T=iK\sigma_y$

$$H(k_{\|},k_z)=H_0+H_1+H_2$$

$H_0=c_0-m_0\tau_z$ Band Inversion, $\mathbb{Z}_2=\mathrm{sgn}(-m_0)$

$H_1=v_z k_z \tau_y + v_{\|}\left(k_y\sigma_x - k_x\sigma_y\right)\tau_x$ Mixing ($\propto$ k)

$H_2=c_z k_z^2 + c_{\|}k_{\|}^2 + \left(m_z k_z^2 + m_{\|}k_{\|}^2\right)\tau_z$ Band Curvature

More precisely

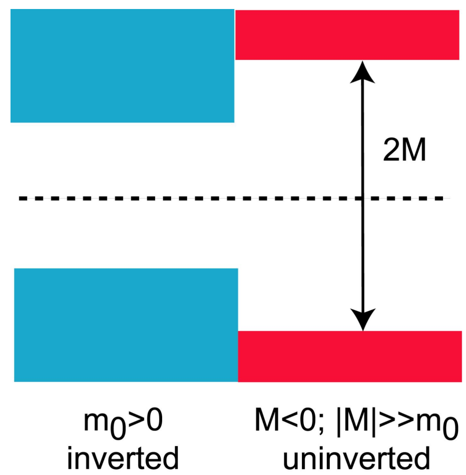
This 3D extension of this idea is subtle.

Most properties of the edge modes (energy in gap, spin structure, influence of bulk anisotropy, sensitivity to surface localized potentials, etc.) are accessible in the four band theory but require a specification of the **boundary condition** that terminates the bulk Hamiltonian.

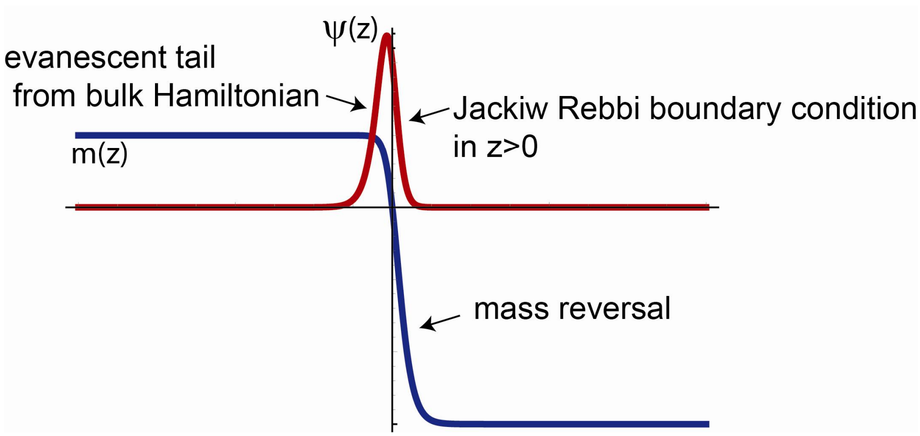
For an **ideal** termination of a 3D TI this is given by a "topological boundary condition." For **nonideal** terminations this is augmented by a two-parameter family of surface localized potentials constrained by P and T symmetries.

Fan Zhang, Kane and GM (2012)

Topological Boundary Condition I



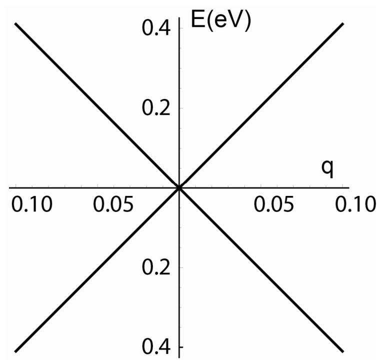
Topological interface is characterized by a mass inversion at the TI surface. Four-band degrees of freedom boosted to mass scale M.

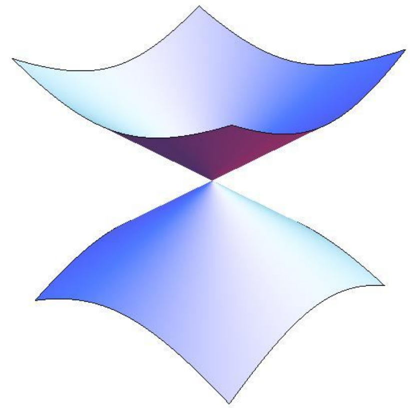


For $M \gg m_0$ exterior wf specifies termination condition for bulk evanescent waves.

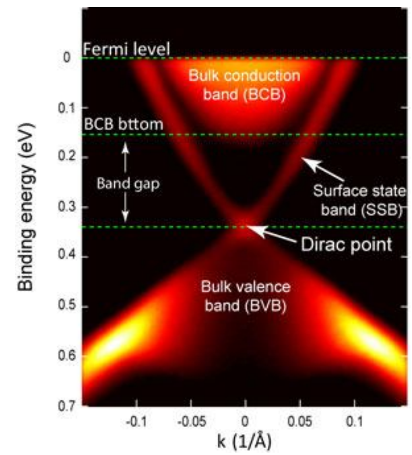
Surface State Hamiltonian

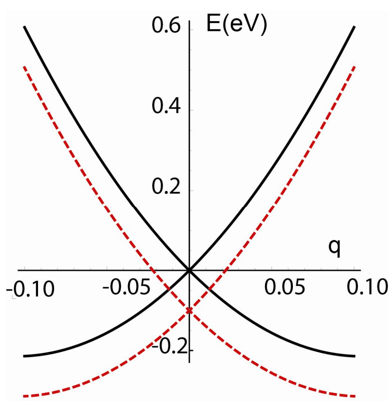
The primitive theory of the (001) surface: $H_{surf} = v_{\parallel}\left(k_y\sigma_x - k_x\sigma_y\right)$

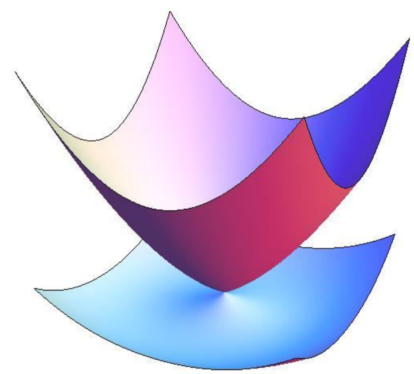




Inherits important quadratic terms that break e-h symmetry and shift the Kramers point from the midgap

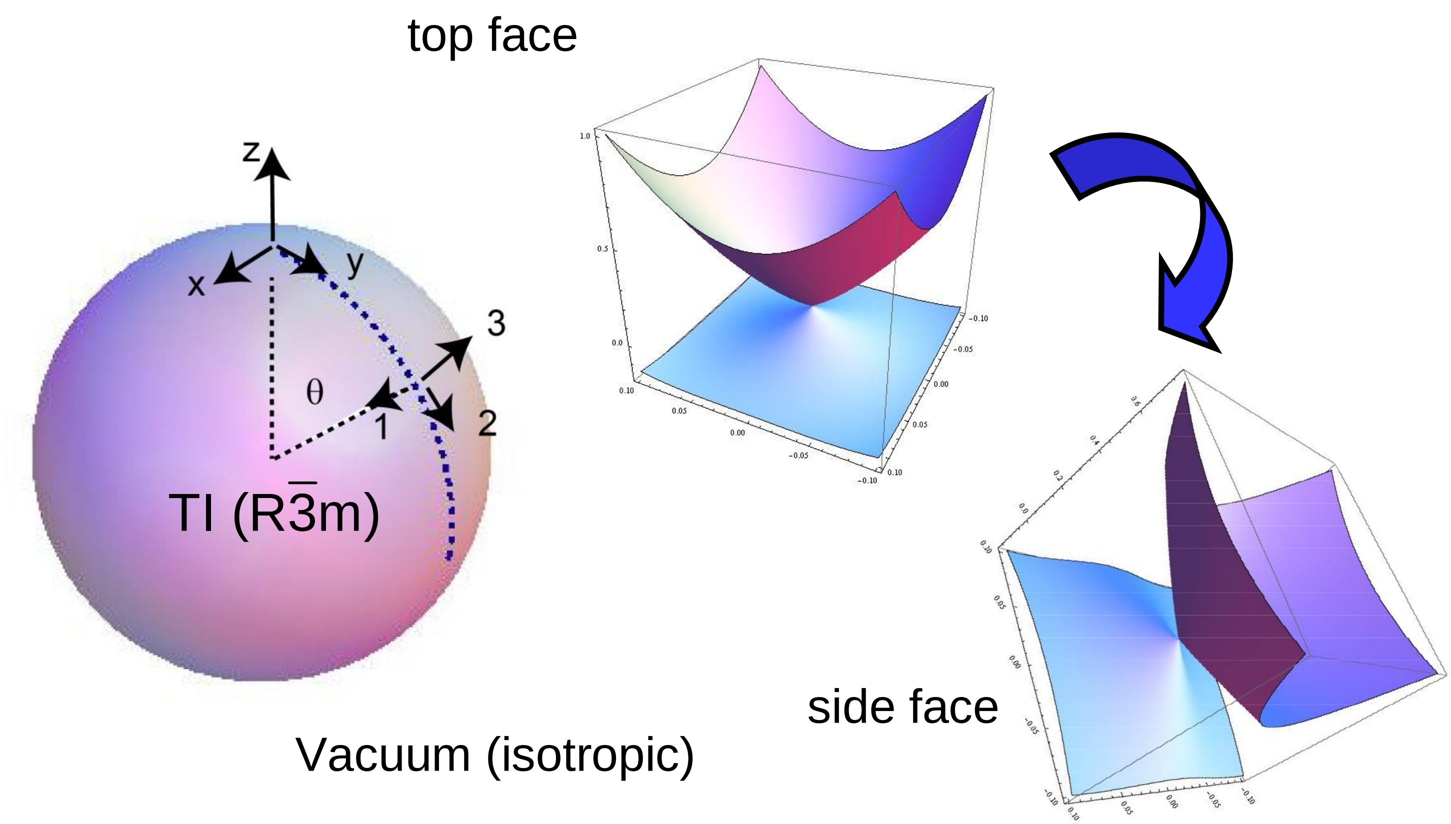






Crystal Face Dependence

These effects are both strong and crystal face dependent because of the anisotropy of the bulk Hamiltonian



Structure of four band model

Fan Zhang, Kane and GM (2012)

(001) Surface (cleavage plane)

In $\tau \otimes \sigma$ representation midgap solution is symmetric under σ-rotations

General surface has $\vec{S}_1 \otimes \vec{S}_2$ structure!

$$\vec{S}_1 = \left\{ \alpha\tau_x + \beta\sigma_y\tau_y, \alpha\tau_y - \beta\sigma_y\tau_x, \tau_z \right\} \quad (\tau\text{-like})$$

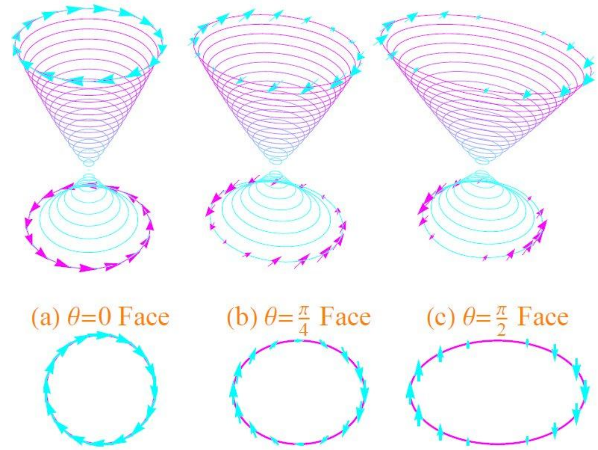
$$\vec{S}_2 = \left\{ \alpha\tau_x - \beta\sigma_z\tau_z, \sigma_y, \alpha\sigma_z + \beta\sigma_x\tau_z \right\} \quad (\sigma\text{-like})$$

$$\alpha = \frac{v_z \cos\theta}{\sqrt{(v_z \cos\theta)^2 + (v_{||} \sin\theta)^2}}$$

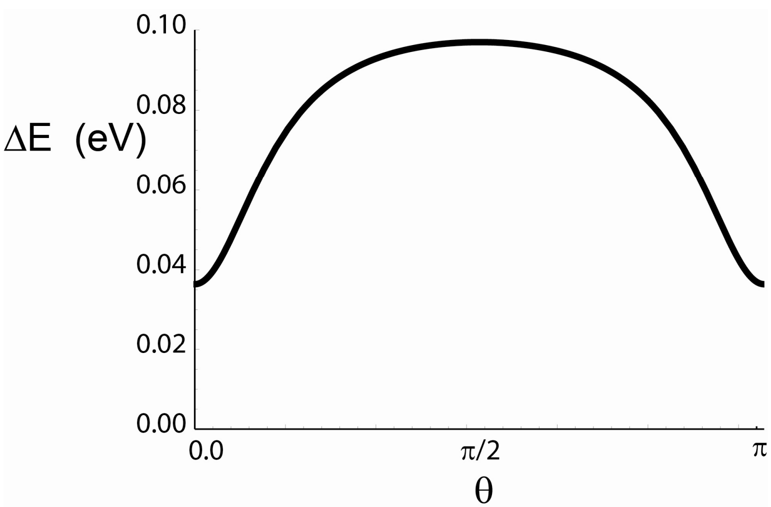
$$\beta = \frac{v_{||} \sin\theta}{\sqrt{(v_z \cos\theta)^2 + (v_{||} \sin\theta)^2}}$$

Face-dependent Dirac physics

Anisotropy in bulk SO coupling
determines spin texture of
its protected surface mode



And the energy of the DP



self doping at step edges

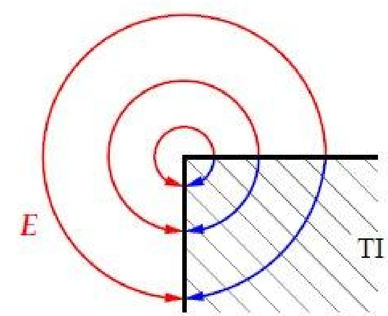


FIG. 2: Electric field near the edge of an anisotropic TI.

Hexagonal warping and spin texture

$$H_{surf} = v_{\|}\left(k_y\sigma_x - k_x\sigma_y\right) + \lambda\left(k_+^3 + k_-^3\right)\sigma_z$$

Symmetry allowed coupling
warps FS (seen) and tips
Spin out of plane on cleavage surface

Chen (2009), Fu (2010), Gedik group (2011)

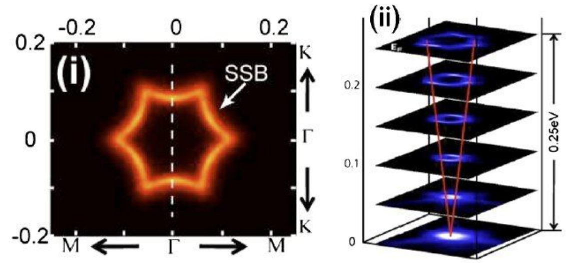
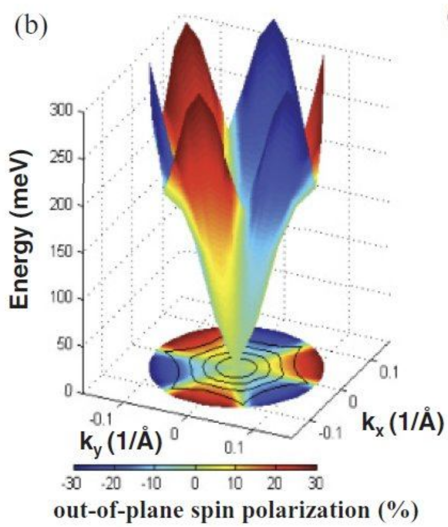
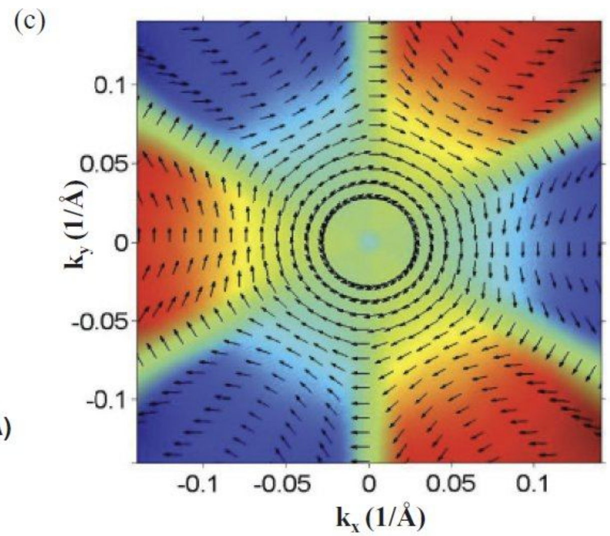
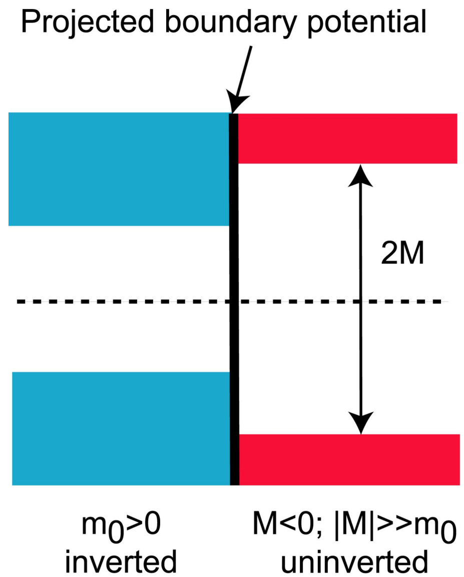


FIG. 1 (color online). (i) Snowflakelike Fermi surface of the surface states on 0.67% Sn-doped Bi_2Te_3 observed in ARPES. (ii) A set of constant energy contours at different energies. From Y. L. Chen *et al.*, Science **325**, 178 (2009). Reprinted with permission from AAAS.

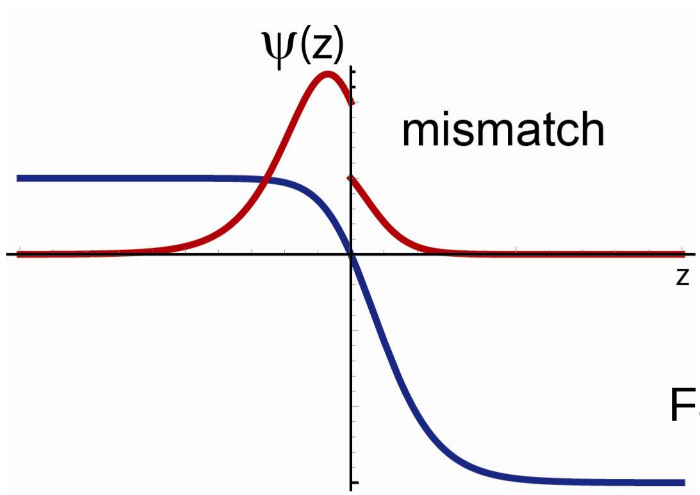




Topological Boundary Condition II



Nonideal interface projected into four-band representation has an additional surface potential that **rotates the wf** of the target state.



J-R boundary condition & **mismatch condition from surface potential** specifies termination of its bulk evanescent states.

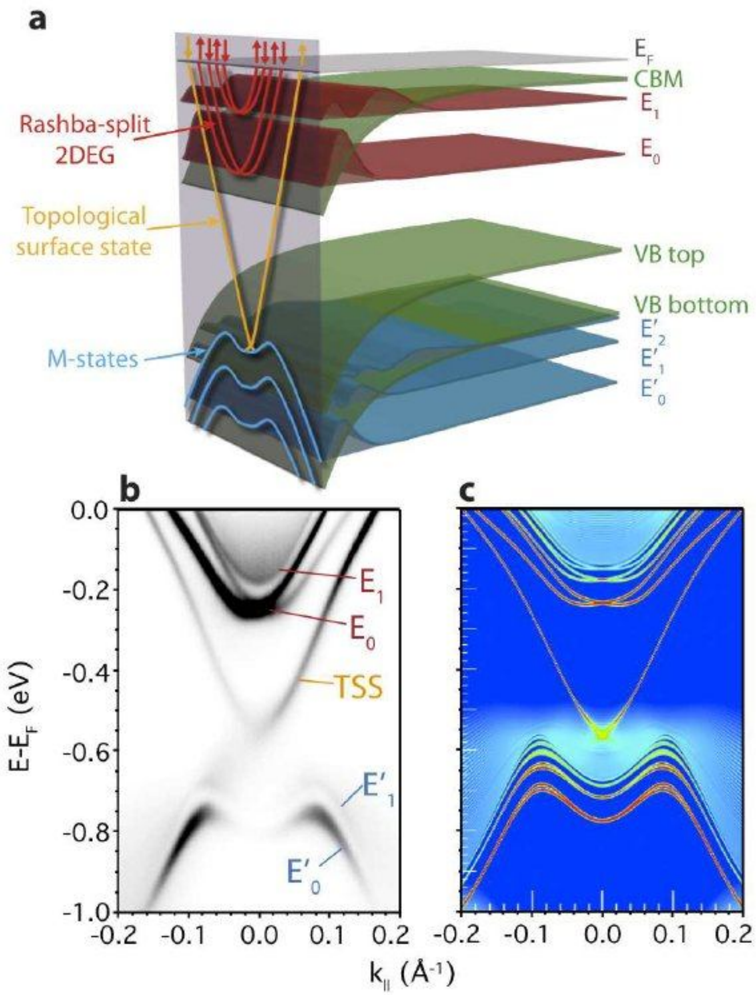
Fan Zhang, Kane and GM (2012)

Quantum well states from band bending

Field effect:
band bending and
quantum confinement

Chemical shift:
differential shift of DP
within gap

Chen et al (2012),
Bahramy et al. (2012)

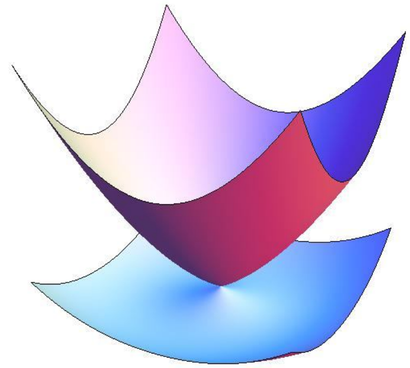


For the surface of a strong topological insulator the SHAPE COUNTS

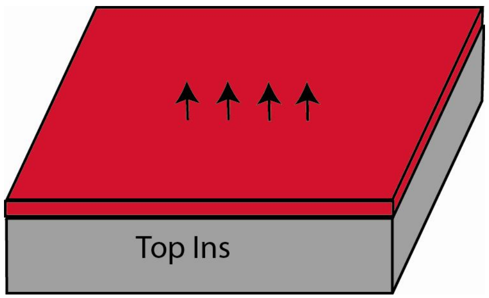
All STI faces support a Dirac node but the orbital and spin texture are nonuniversal and crystal face-dependent

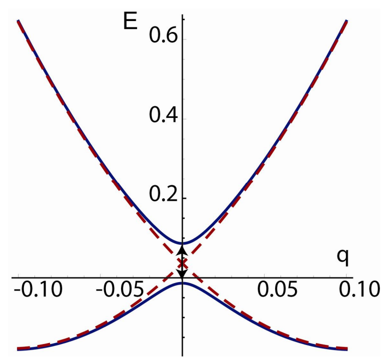
Symmetry Breaking by FM exchange coupling

Kramers TRIM Degeneracy

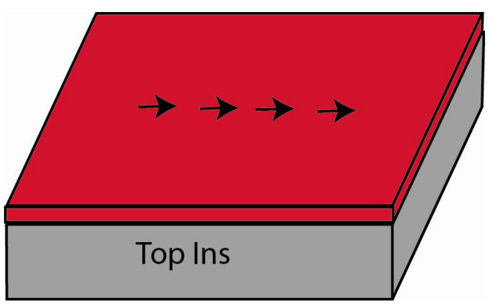


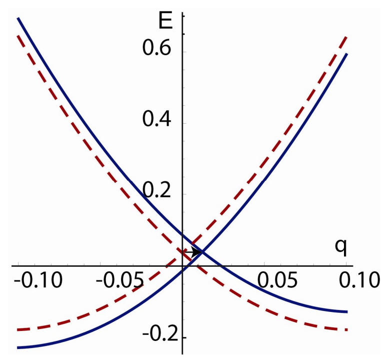
Is removed by $\Delta_\perp \sigma_z$





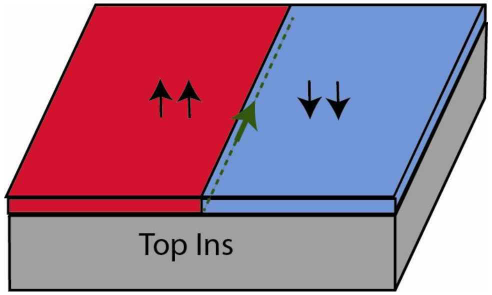
But is shifted by $\Delta_{||} \cdot \sigma_{||}$





1D Chiral Mode along domain wall

Reversing exchange field = mass inversion



Algebra for any noncleavage plane: $\tau \otimes \sigma \to \vec{S}_1 \otimes \vec{S}_2$

$$\Delta_x \sigma_x = \alpha(\theta)\Delta_x S_2^x + \beta(\theta)\Delta_x S_2^z S_1^z$$

$$\Delta_y \sigma_y = \Delta_y S_2^y$$

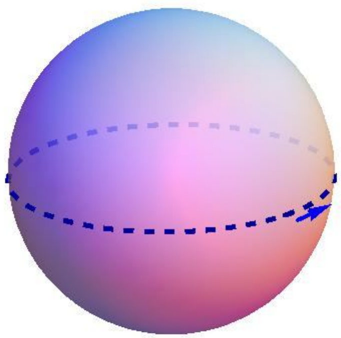
$$\Delta_z \sigma_z = \alpha(\theta)\Delta_z S_2^z - \beta(\theta)\Delta_z S_2^x S_1^z$$

Mass inversion occurs at "edges" for **uniform** exchange field

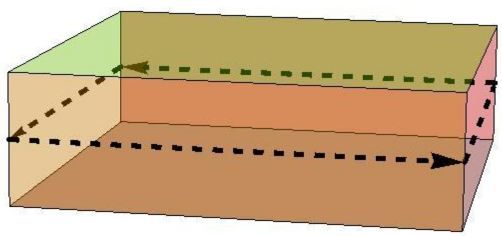
Edge induced 1D Chiral Modes

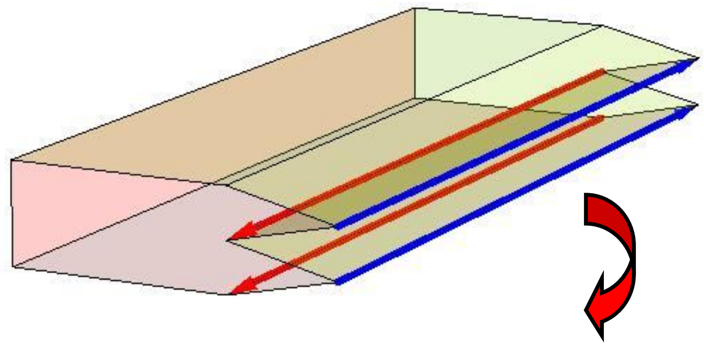
(001) exchange field

sphere

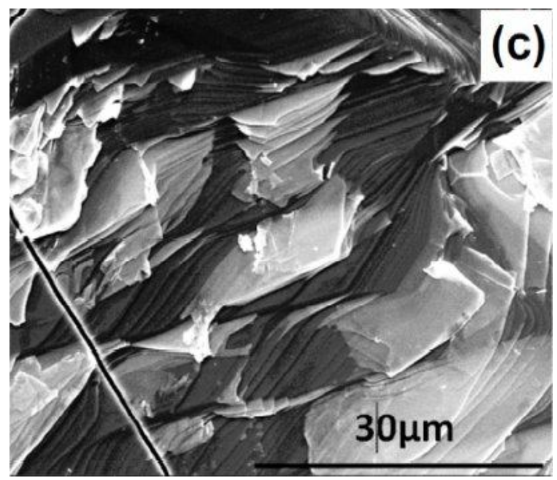


slab





layered



Bi_2Se_3/Fe_4Se_7 intergrowth

Cava (2012)

Mass inversion at side “edges”

Fan Zhang, Kane and GM (2012)

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Four Band Models (second generation)
Fan Zhang, C.L. Kane and E.J. Mele arXiv:1203.6382

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