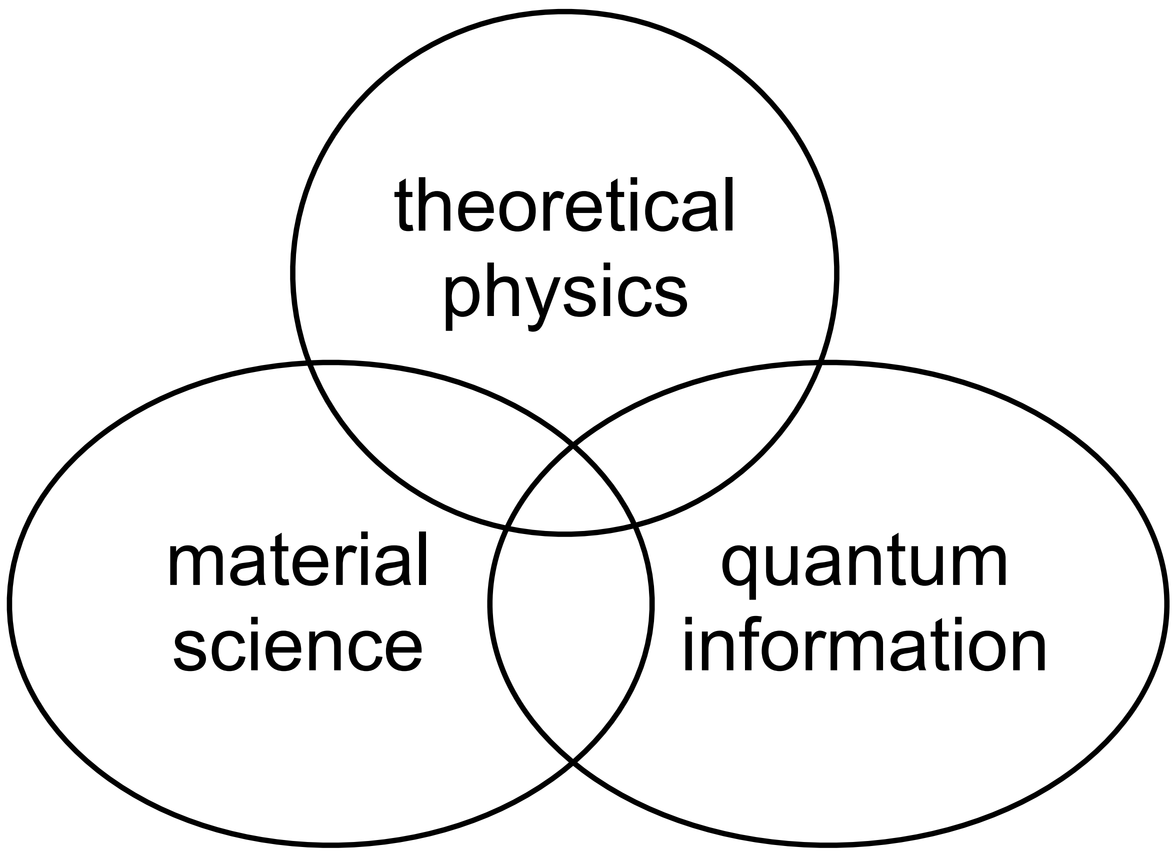
Topological Materials

Liang Fu



Institute of Solid State Physics, Tokyo, 06/03/13

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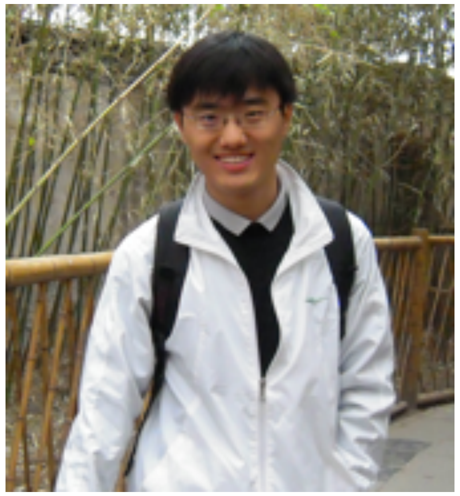

Junwei Liu
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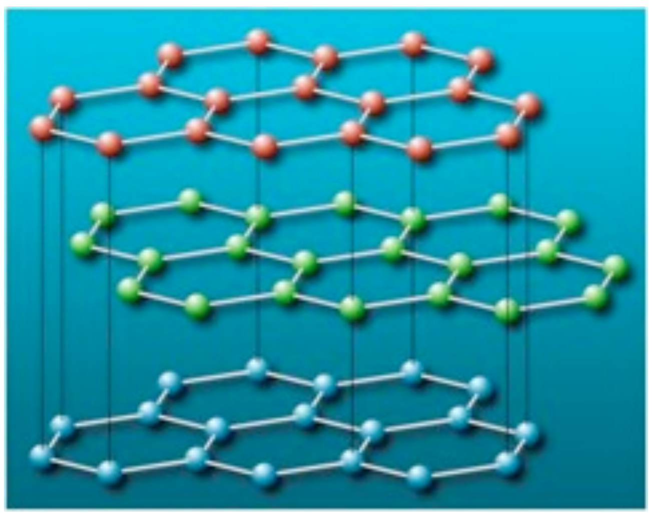
Simple View of Solids

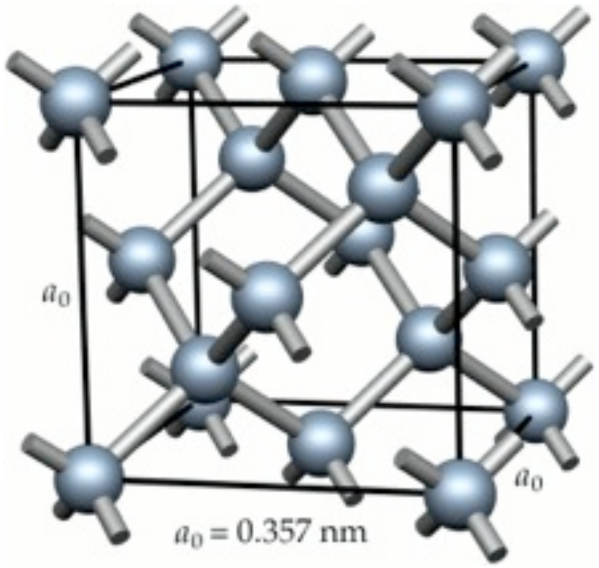
- a local perspective based on orbitals and bonds

Graphite



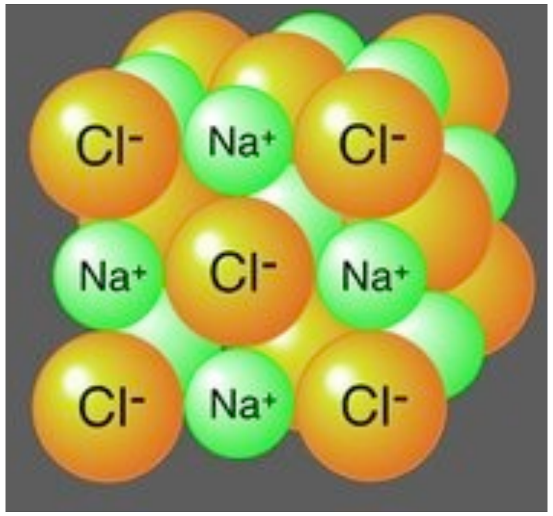
$C: 2s^1 2p^3 \Rightarrow sp^2 + p_z$

Diamond



$C: 2s^1 2p^3 \Rightarrow sp^3$

NaCl



$Na(3s^1) + Cl(3p^5) \Rightarrow Na^+Cl^-$

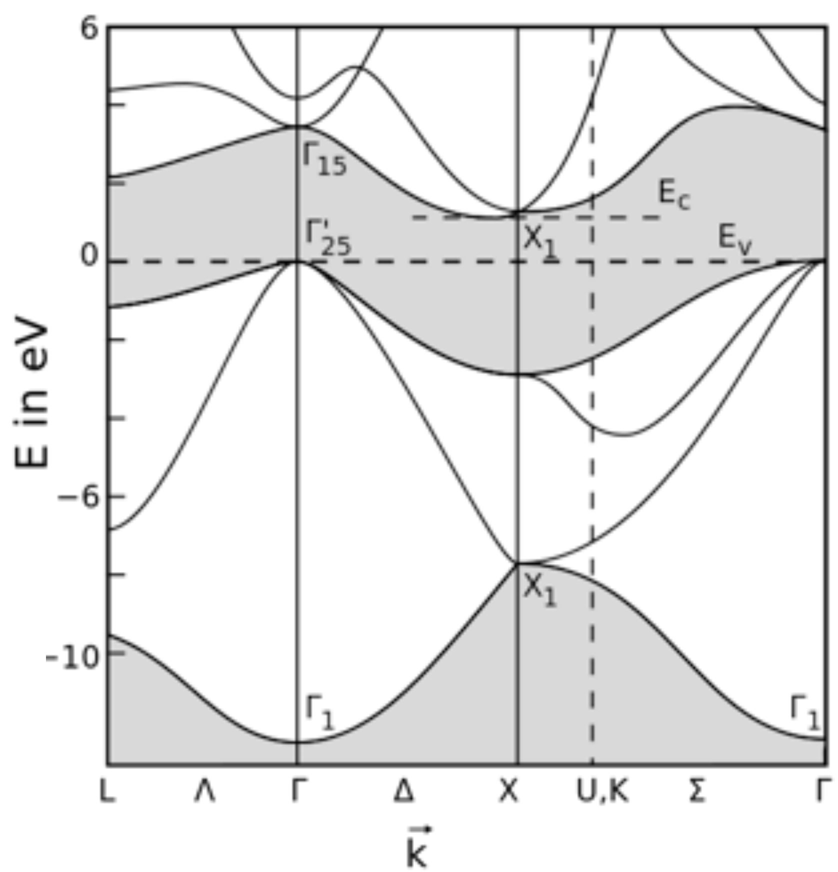
- empirical relation between structure and property

  diamond ≈ silicon ≈ germanium ≠ graphite; NaCl ≈ KCl

Band Theory of Solids

- electron in solids forms itinerant Bloch wave in periodic potential
- band insulators: a finite energy gap between occupied and empty states

silicon



$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

k : crystal momentum

$u_{\mathbf{k}}$: wavefunction within a unit cell

$$H(\mathbf{k}) = \frac{(\hat{\mathbf{P}} - \hbar\mathbf{k})^{\mathbf{2}}}{2m} + U(\hat{\mathbf{r}})$$

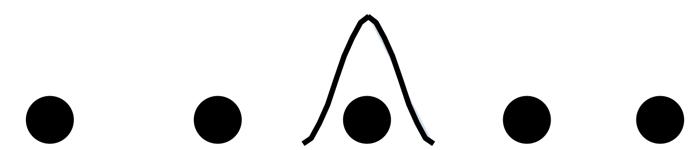
$$H(\mathbf{k}) u_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})$$

The Same or Not The Same

Band theory: a global structure

Orbital: local approach

Wannierization



$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j}\phi_j(\mathbf{r})$$

$$\text{Det}\begin{pmatrix} \psi_{k_1}(r_1) & \psi_{k_2}(r_1) & \ldots \\ \psi_{k_1}(r_2) & \psi_{k_2}(r_2) & \ldots \\ . & . & . \end{pmatrix} = \text{Det}\begin{pmatrix} \phi_1(r_1) & \phi_2(r_1) & \ldots \\ \phi_1(r_2) & \phi_2(r_2) & \ldots \\ . & . & . \end{pmatrix}$$

For most solids, locality is restored in band theory by transforming Bloch waves to Wannier functions, the analog of atomic orbitals.

The Same or Not The Same: Question of Topology

Topology: property of a manifold that is insensitive to smooth deformations.

 $\neq$  $=$ 

(g=1) (g=0)

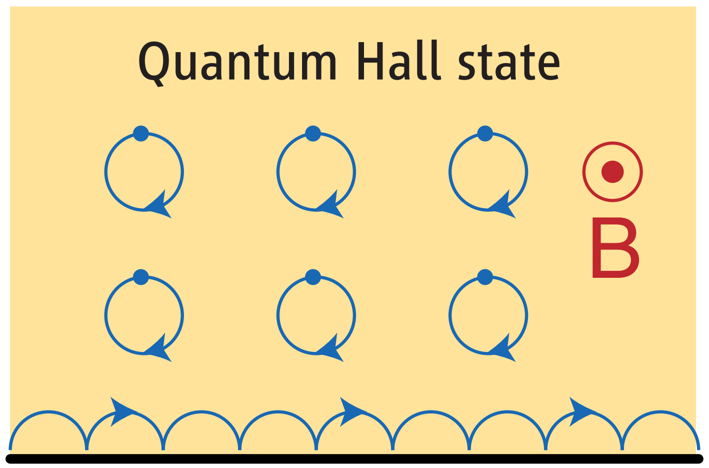
Example: genus (g) is an integer topological invariant of 2D surfaces.

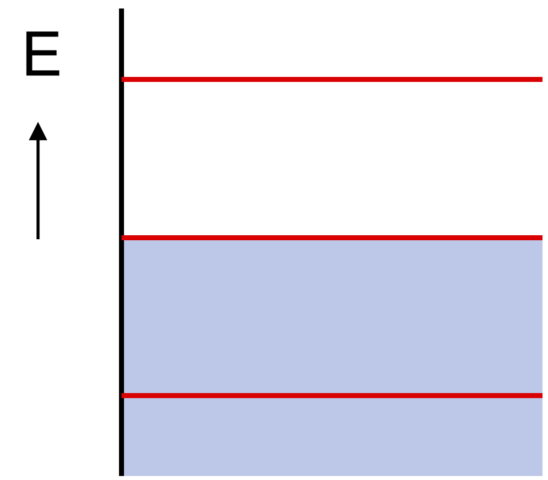
Topology of electronic solids:

Question: are all gapped insulators adiabatically connected?

To answer this question requires understanding topology of occupied wavefunctions $u_{\mathbf{k}}(\mathbf{r})$ in the Brillouin zone, which form a manifold in Hilbert space.

Quantum Hall Effect and Topological States of Matter





Hall conductivity is quantized when chemical potential lies within the gap.

$\sigma_{xy}=N\,e^2/h$: only a thermodynamic principle can explain this accuracy.

(Laughlin)

Hall conductivity is a topological invariant of ground state wavefunction.

(TKNN, 1982)

Kubo formula: $$\sigma_{xy} = \frac{i}{2\pi}\int d^2k\,\epsilon_{\mu\nu}\langle\partial_\mu u_k|\partial_\nu u_k\rangle = n$$

Topology and Modern Band Theory

Global structure of band theory has more to offer:

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

(Haldane, 1987)

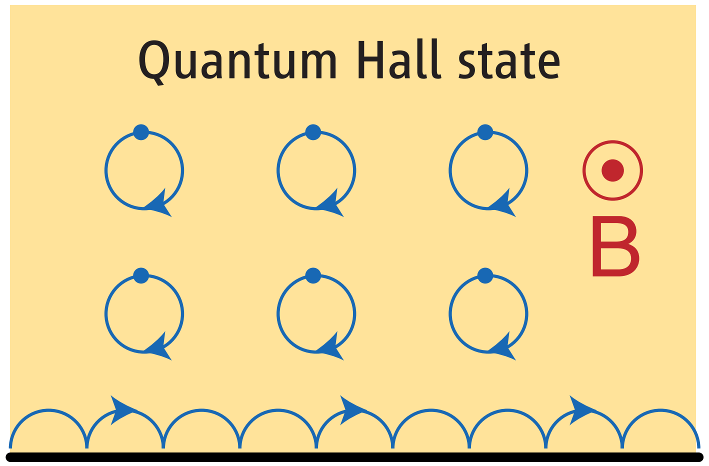
Chern insulator: topological state of matter

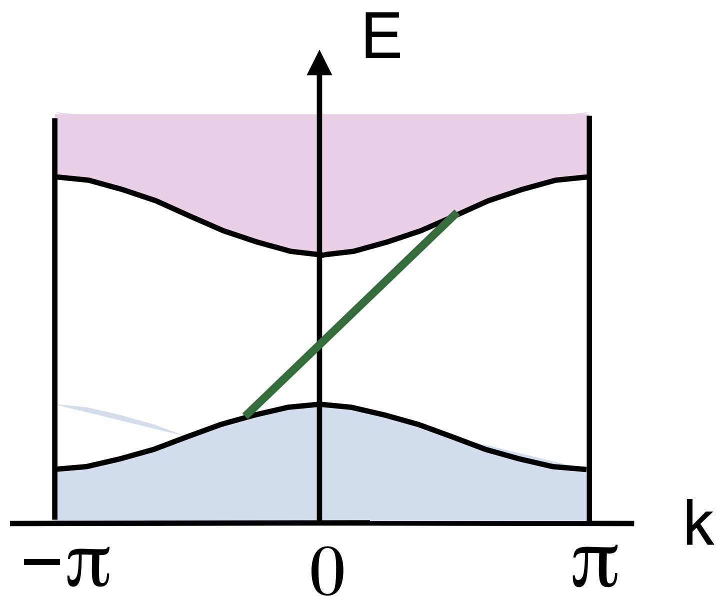
- topologically distinct from conventional insulators
- nontrivial band carries Chern number
- experimental observation (Chang et al, 2013)

Breakdown of local approach: no localized Wannier function

Edge States: Consequence of Topology

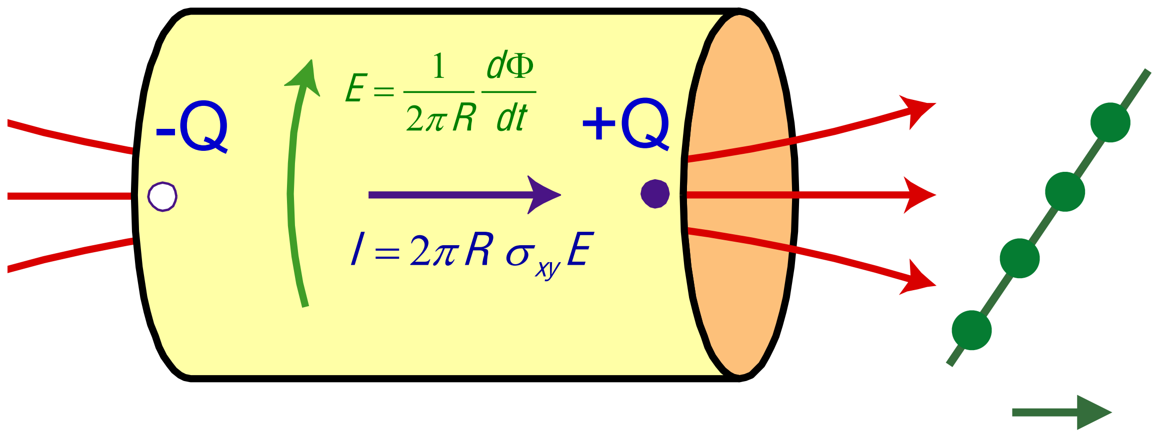
Change of topological invariant is accompanied by gap-closing.





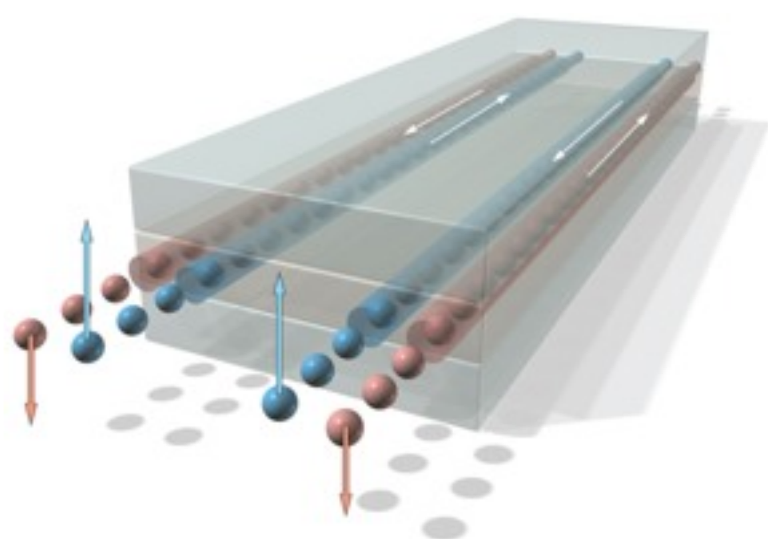
Quantum Hall edge states:

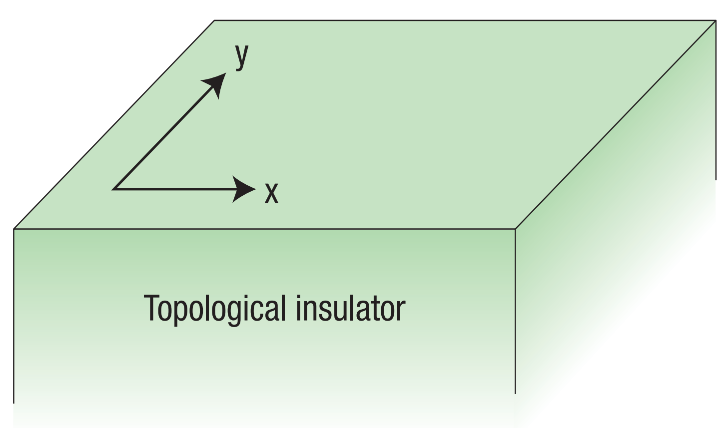
- one-way moving
- chiral anomaly
- cannot be realized in any 1D wire.

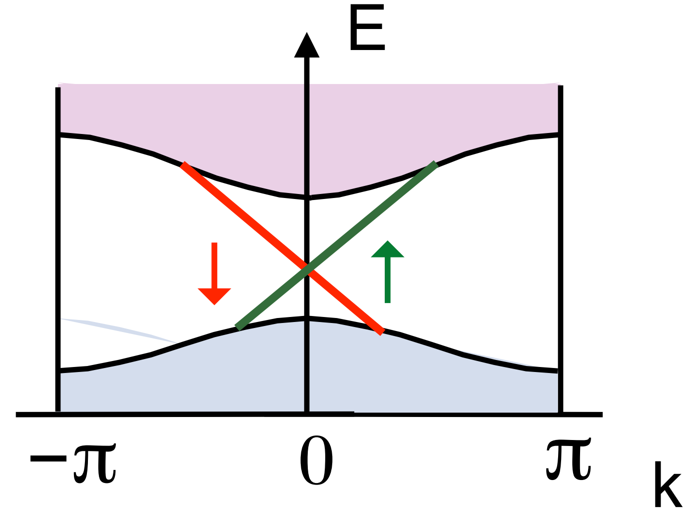


Topological Insulators

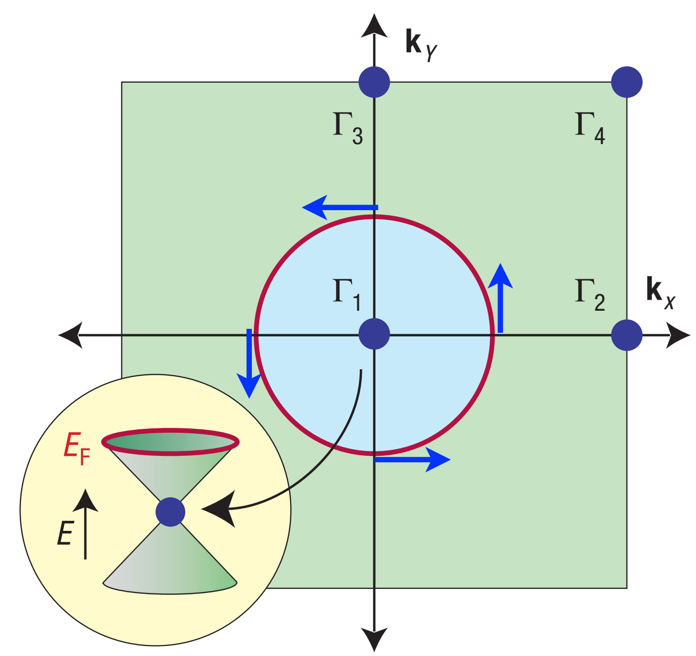
topology meets symmetry







Kramers degeneracy



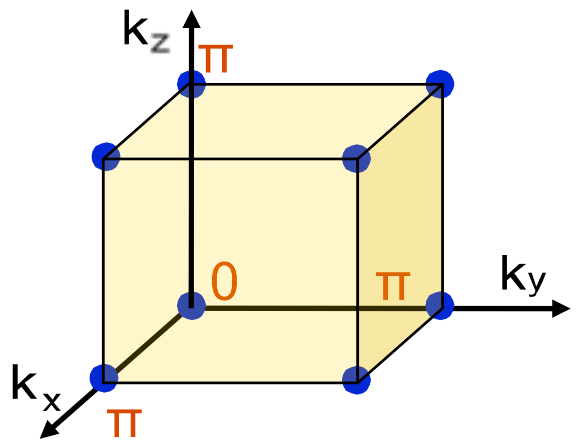
- topological distinction requires time-reversal symmetry
- helical surface states with odd # of Dirac points
- time-reversal anomaly: avoids fermion doubling

Kane & Hasan, RMP 10
Qi & Zhang, RMP 11

Z_2 Topological Invariant & Parity Criterion

Explicit formula for topological invariant: (Kane & Mele; LF & Kane; Moore & Balents ...)

$$(-1)^\nu = \prod_{i=1}^{4} \frac{\mathrm{Pf}[w(\Gamma_i)]}{\sqrt{\det[w(\Gamma_i)]}} = \pm 1 \qquad w_{mn} = \langle u_m(k)|\Theta|u_n(-k)\rangle$$



- computation requires a smooth gauge
- ab-initio implementation

(Soluyanov & Vanderbilt, Dai et al ...)

Parity criterion: LF & Kane, PRB 76, 045302 (2007)

- choose a canonical gauge for inversion-symmetric insulators:

$$|u_i(\mathbf{k})\rangle = \epsilon_{ij}\Xi|u_j(\mathbf{k})\rangle \qquad \Xi = P\Theta$$

- fixed-point formula:

$$(-1)^\nu = \prod_i \prod_n \xi_{2n}(\Gamma_i)$$

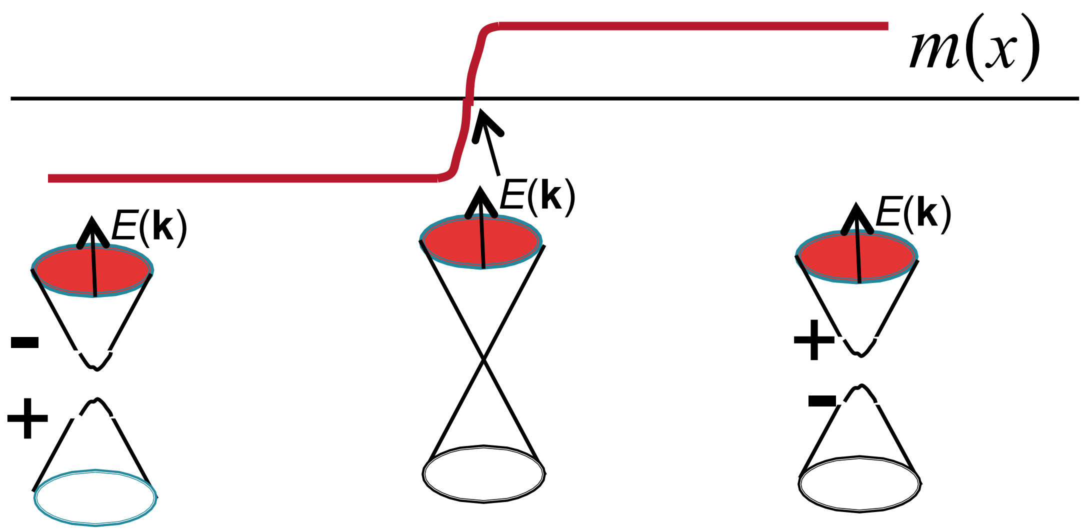
(Z_2 invariant = parity of occupied bands)

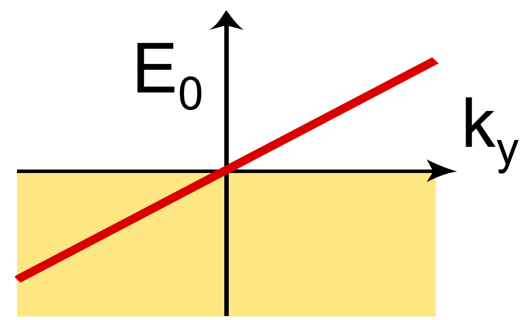
Origin of Topological Insulators: Parity Inversion

Gap-closing transition is generically described by four-component Dirac theory

$$H = \psi^\dagger(-iv_F\partial_j\Gamma_j\psi + m\Gamma_0)\psi$$

	P	T
Γ_0	+	+
$\Gamma_{1,\dots 4}$	-	-



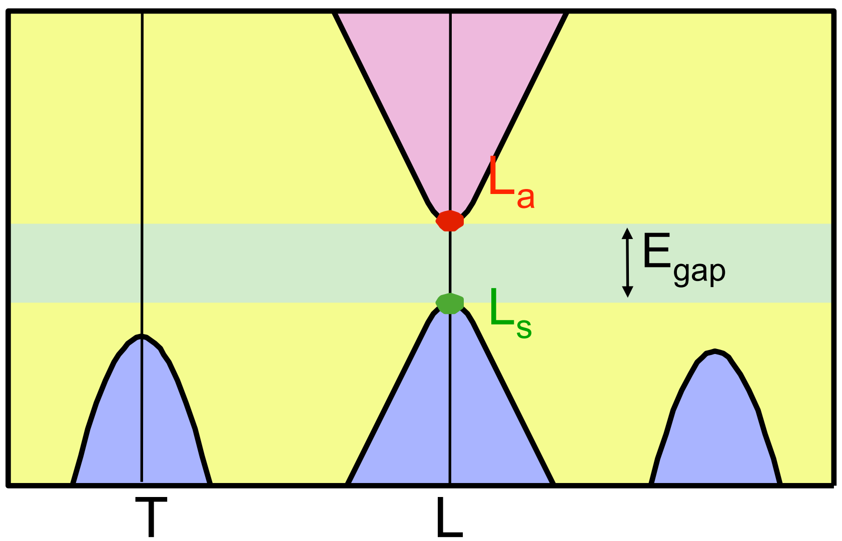


- only <u>one</u> mass term is allowed in P and T symmetric materials
- parity operator = Dirac mass; parity inversion = mass reversal
- TI surface = massless domain wall fermion

$$\psi_{q_x}(x, y) \propto e^{iq_x x} e^{-\int_0^y dy' m(y') dy' / v_F}$$

From Parity Criterion to Material Prediction

Bi-Sb alloy



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					$(1;111)$

Prediction: Bi-Sb, strained HgTe and etc are 3D topological insulators. (LF & Kane 07)

From Parity Criterion to Material Prediction

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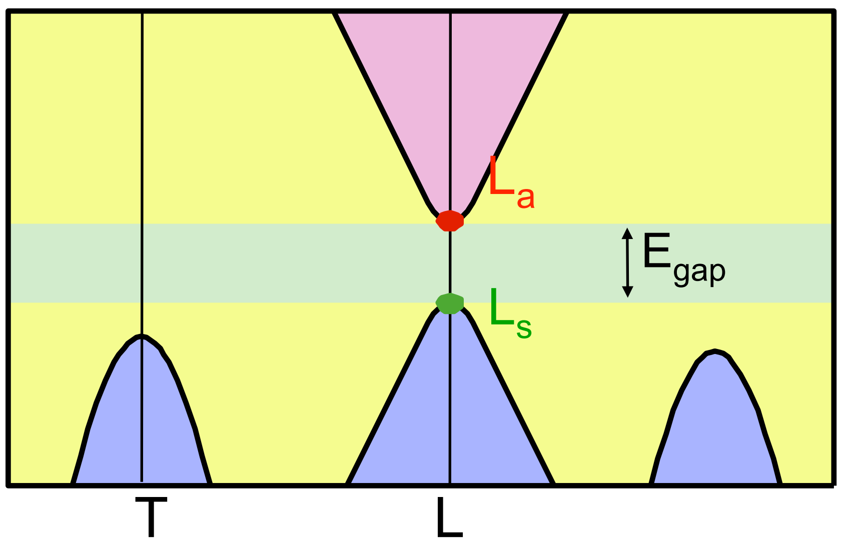

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$3L$	L_s L_a L_s L_a L_s	$+$
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$1T$	T_6^- T_6^+ T_6^- T_6^+ T_{45}^-	$-$
	Z_2 class	$(1;111)$

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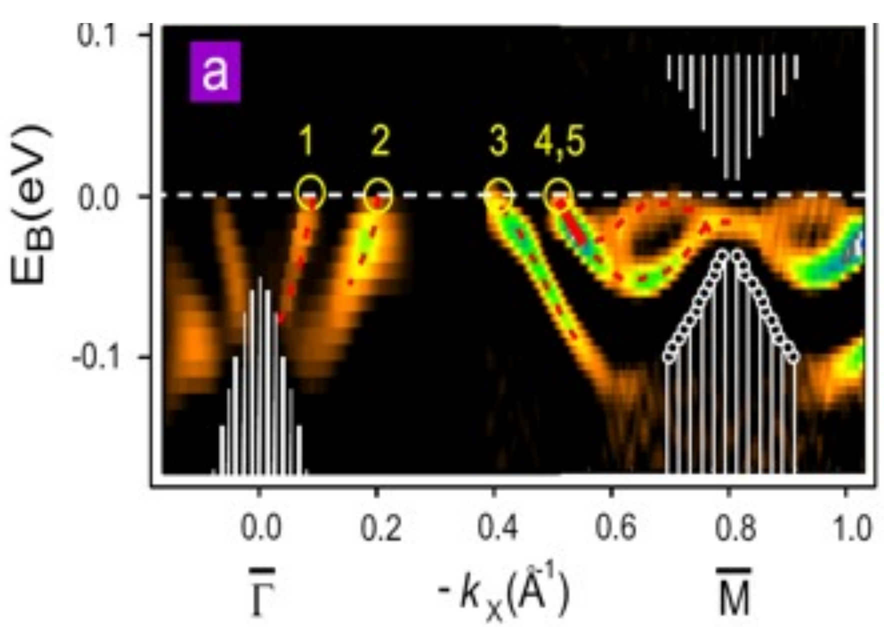
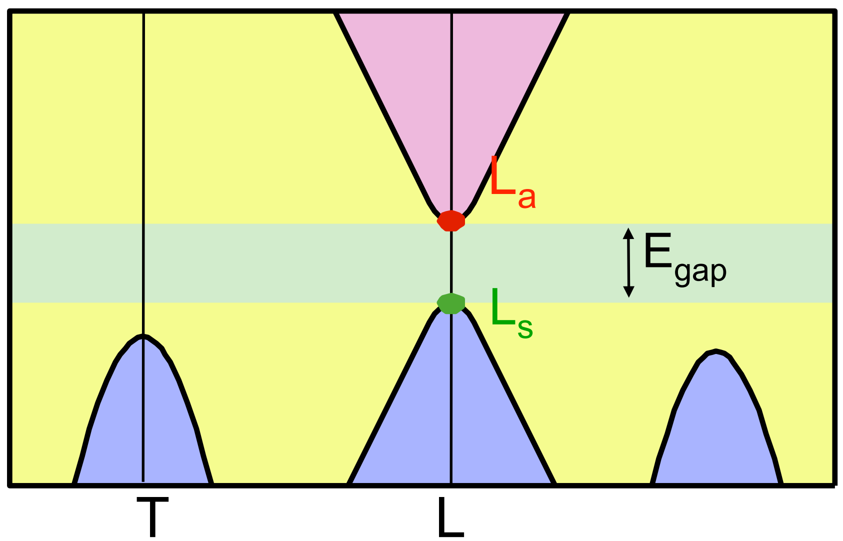
Bi-Sb (111) surface



(Hsieh et al 08)

From Parity Criterion to Material Prediction

Bi-Sb alloy



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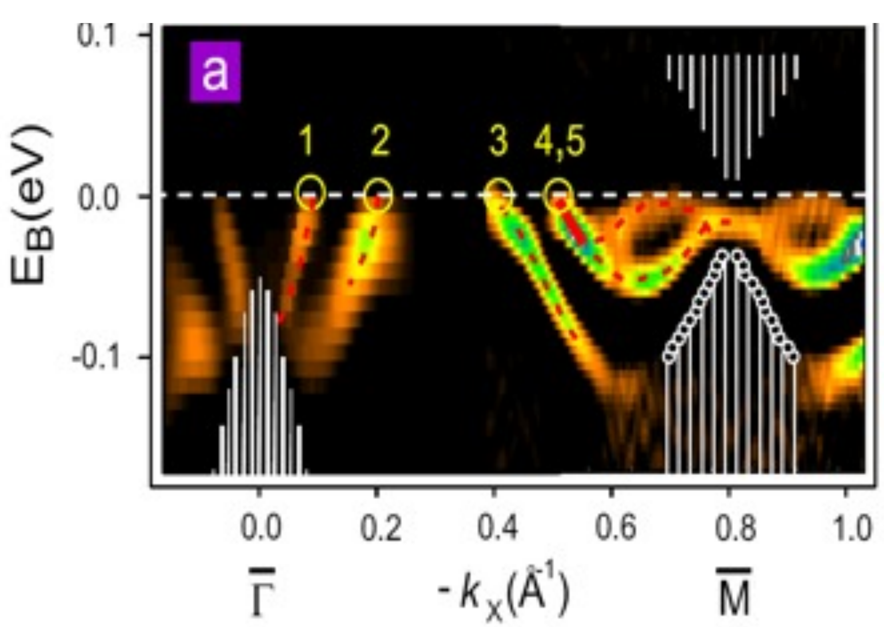
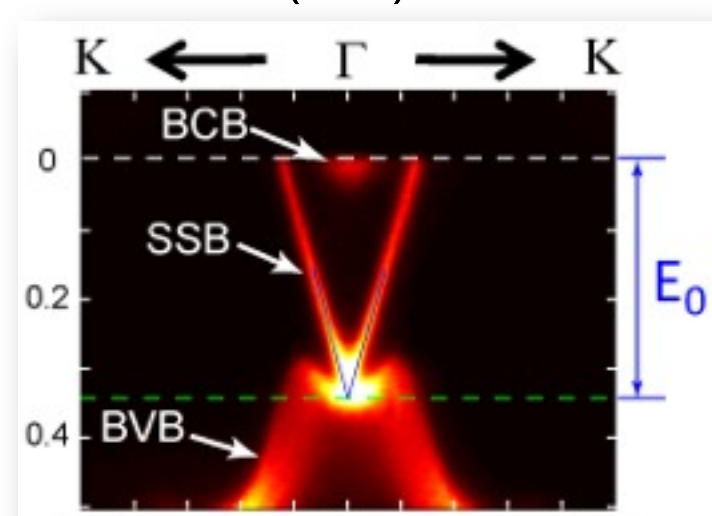


(Hsieh et al 08)

Bi_2Te_3 (111) surface



(expt: Chen et al 09;
theory: Zhang et al 09)

Topology meets Crystallography

Crystal symmetry (point group) is a defining property of periodic solids.

Question: for a given crystal symmetry, are there topologically distinct types of energy bands with the same symmetry labels?

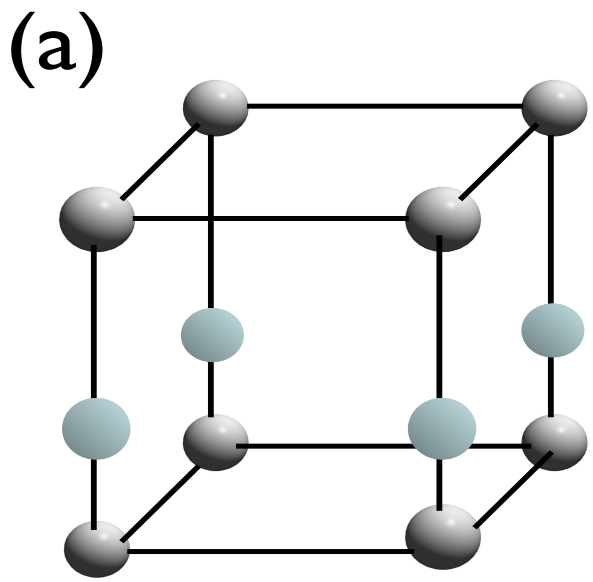
e.g., can s- and p-orbitals in diamond lattice generate a band structure different from silicon?

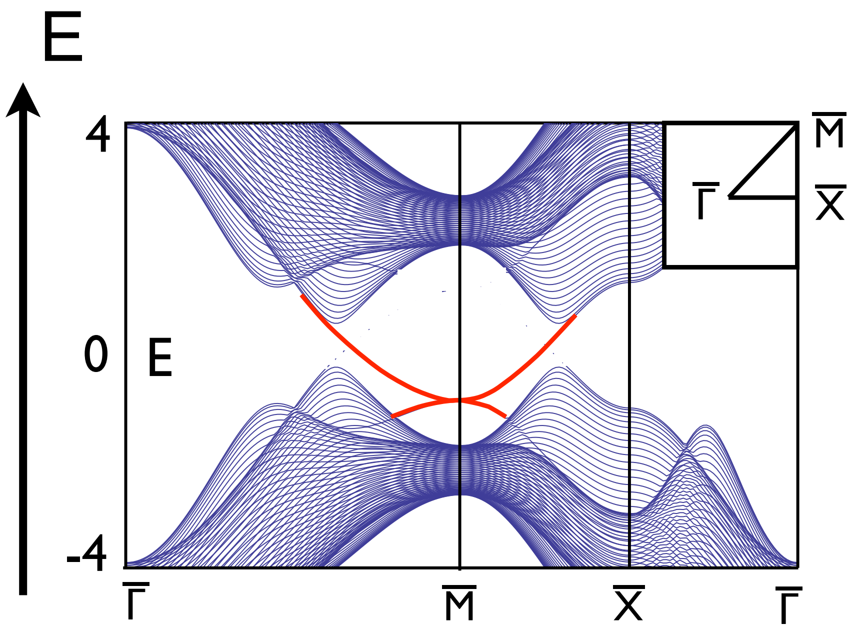
Beyond structure-property relation?

Topological Crystalline Insulators

Proof of principle: LF, PRL 106, 106802 (2011).

a model of p_x and p_y orbitals in tetragonal lattice with C_4 symmetry

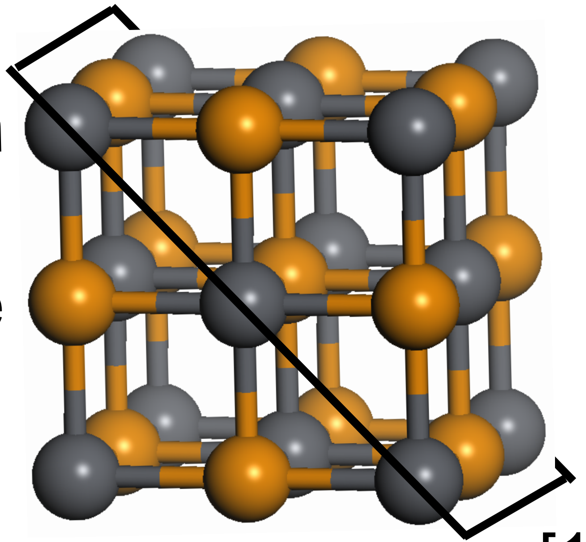




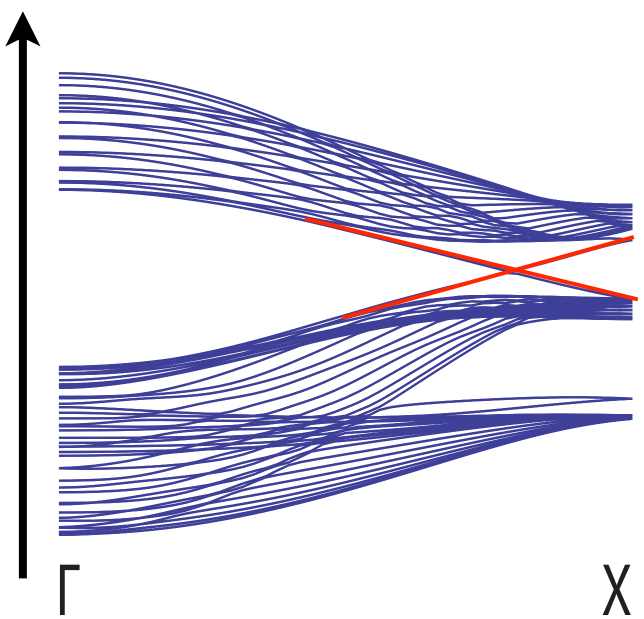
- trivial phase = occupied states on a given sublattice
- a nontrivial phase: characterized by a new Z_2 invariant (orientability)
- protected metallic states on symmetry-preserving surfaces

=> proves the existence of topological crystalline insulators

Prediction: Topological Crystalline Insulators in the SnTe Material Class



$$H_{\text{tb}} = m\sum_{j}(-1)^{j}\sum_{\mathbf{r},\alpha}\mathbf{c}^{\dagger}_{j\alpha}(\mathbf{r})\cdot\mathbf{c}_{j\alpha}(\mathbf{r})$$
$$+\sum_{j,j'}t_{jj'}\sum_{(\mathbf{r},\mathbf{r}'),\alpha}\mathbf{c}^{\dagger}_{j\alpha}(\mathbf{r})\cdot\hat{\mathbf{d}}_{\mathbf{rr}'}\,\hat{\mathbf{d}}_{\mathbf{rr}'}\cdot\mathbf{c}_{j'\alpha}(\mathbf{r}')+h.c.$$
$$+\sum_{j}i\lambda_{j}\sum_{\mathbf{r},\alpha,\beta}\mathbf{c}^{\dagger}_{j\alpha}(\mathbf{r})\times\mathbf{c}_{j\beta}(\mathbf{r})\cdot\mathbf{s}_{\alpha\beta}.$$

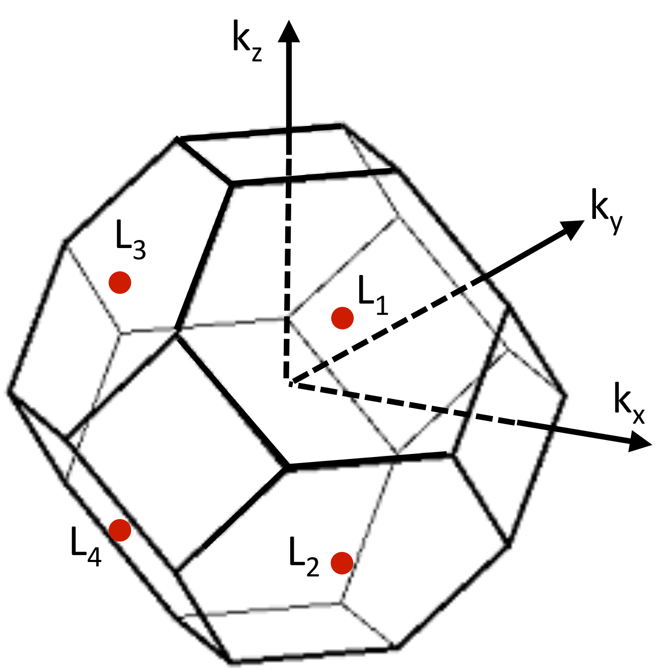


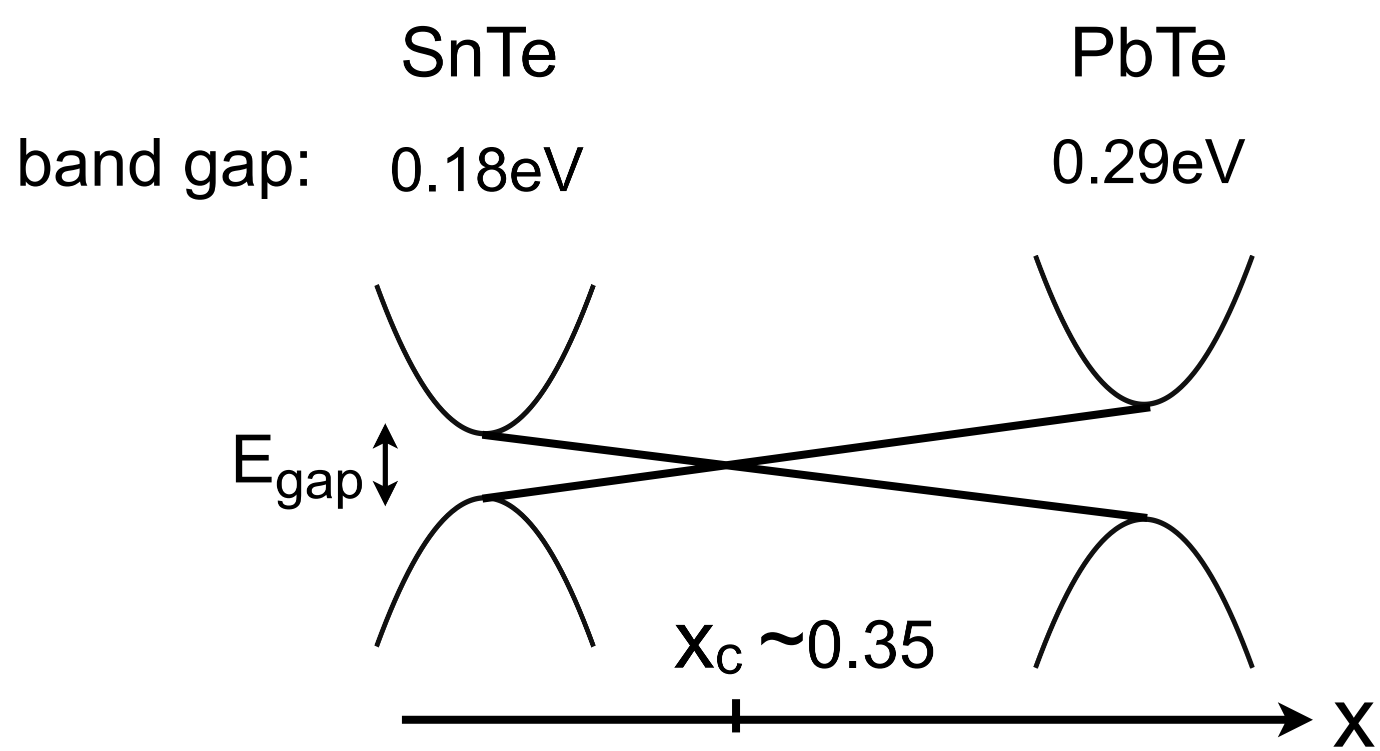
- IV-VI rocksalt semiconductors: SnTe, PbTe, PbSe
- TCI phase in SnTe protected by (110) mirror symmetry

Timothy Hsieh, Lin, Liu, Duan, Bansil & LF, Nature Communications, 2012

Band Inversion between SnTe and PbTe

Band gap of $Pb_{1-x}Sn_xTe$: (Dimmock, Melngailis & Strauss, 1966)

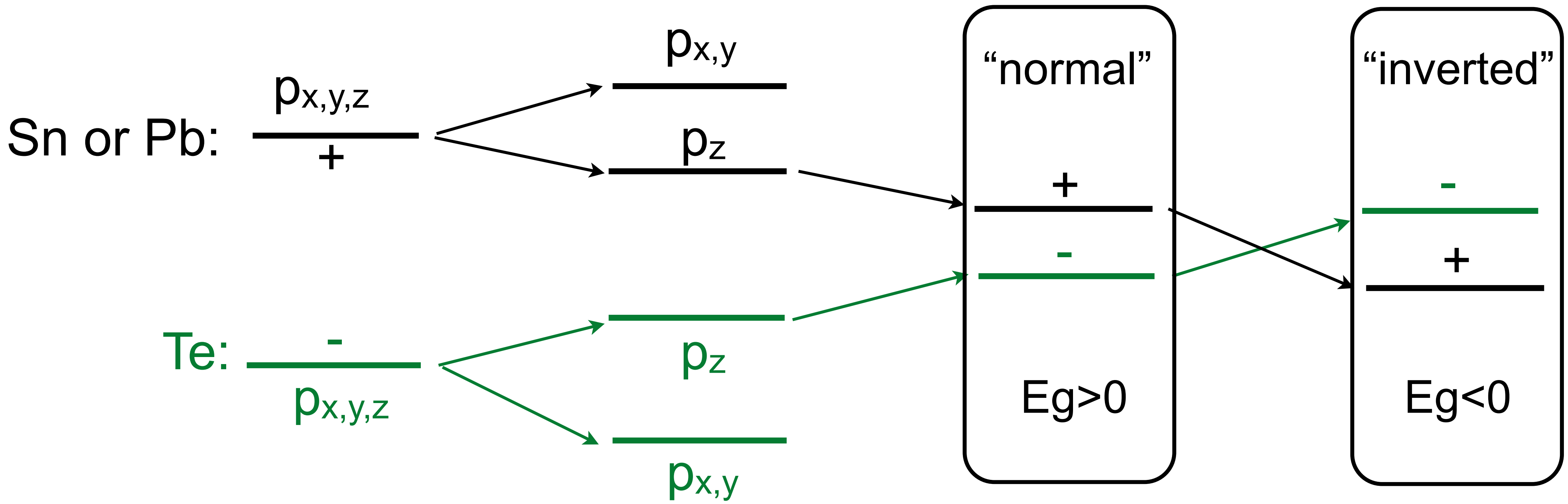




- even number of band inversion at four L points
- neither SnTe nor PbTe is topological insulator (LF & Kane, PRB 07)

Origin of Band Inversion

Energy level diagram at L:



(i) on-site energy + p-orbital hopping (ii) spin-orbit coupling

(ionicity) (covalency)

- two types of band ordering at L:

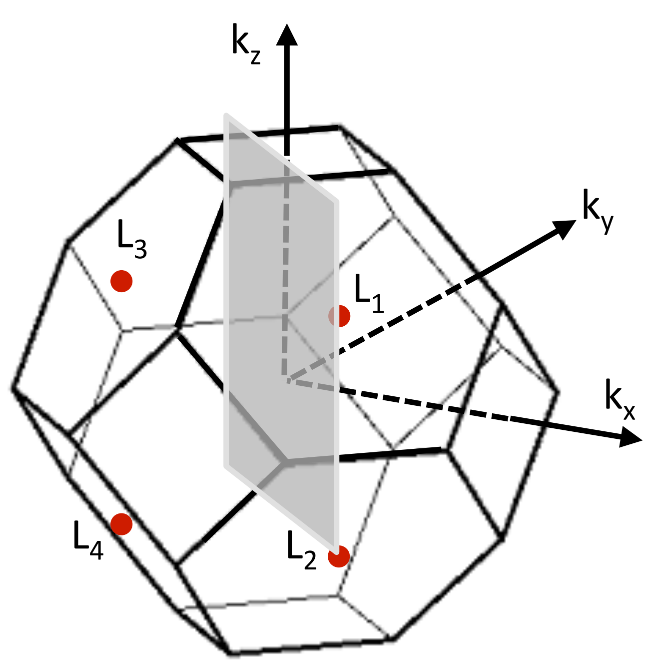
normal = ionic insulator (trivial); inverted = topologically nontrivial ?

Mirror Symmetry and Topology

When (110) mirror symmetry is present, band inversion cannot be avoided and involves a change of band topology.

k.p theory: $$H = m\sigma_z + v(k_x s_y - k_y s_x)\sigma_x + v_z k_z \sigma_y$$

on k_x=0 plane: $$H(k_x = 0) = m\sigma_z - v k_y s_x \sigma_x + v_z k_z \sigma_y$$



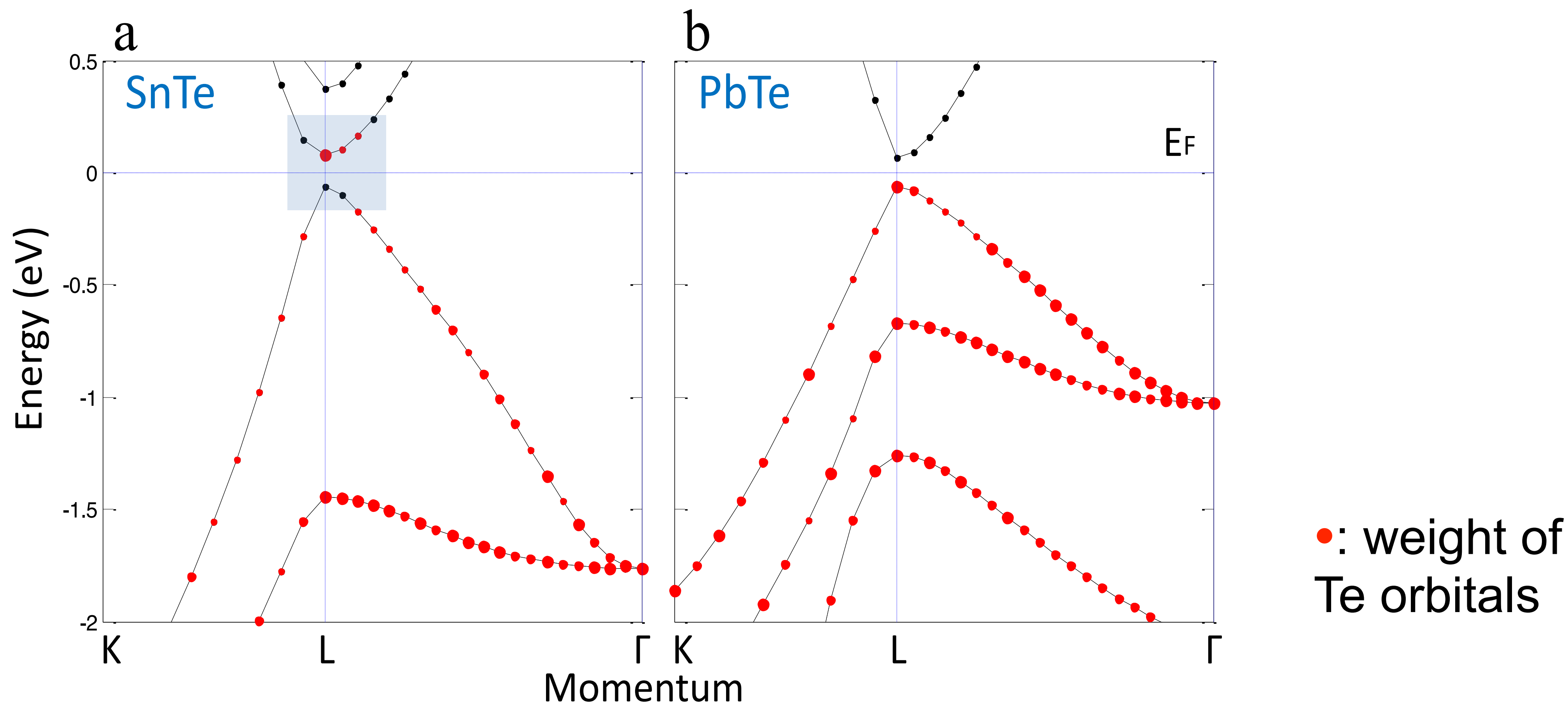
- k_x=0 plane is invariant under reflection w.r.t (110)
- two sets of bands with opposite mirror eigenvalues (s_x =1 and -1)
- Chern number defined for each band separately

(Teo, LF & Kane, PRB 08)

Band inversion at L_1 and L_2 changes Chern number of each band by ±2.

SnTe versus PbTe

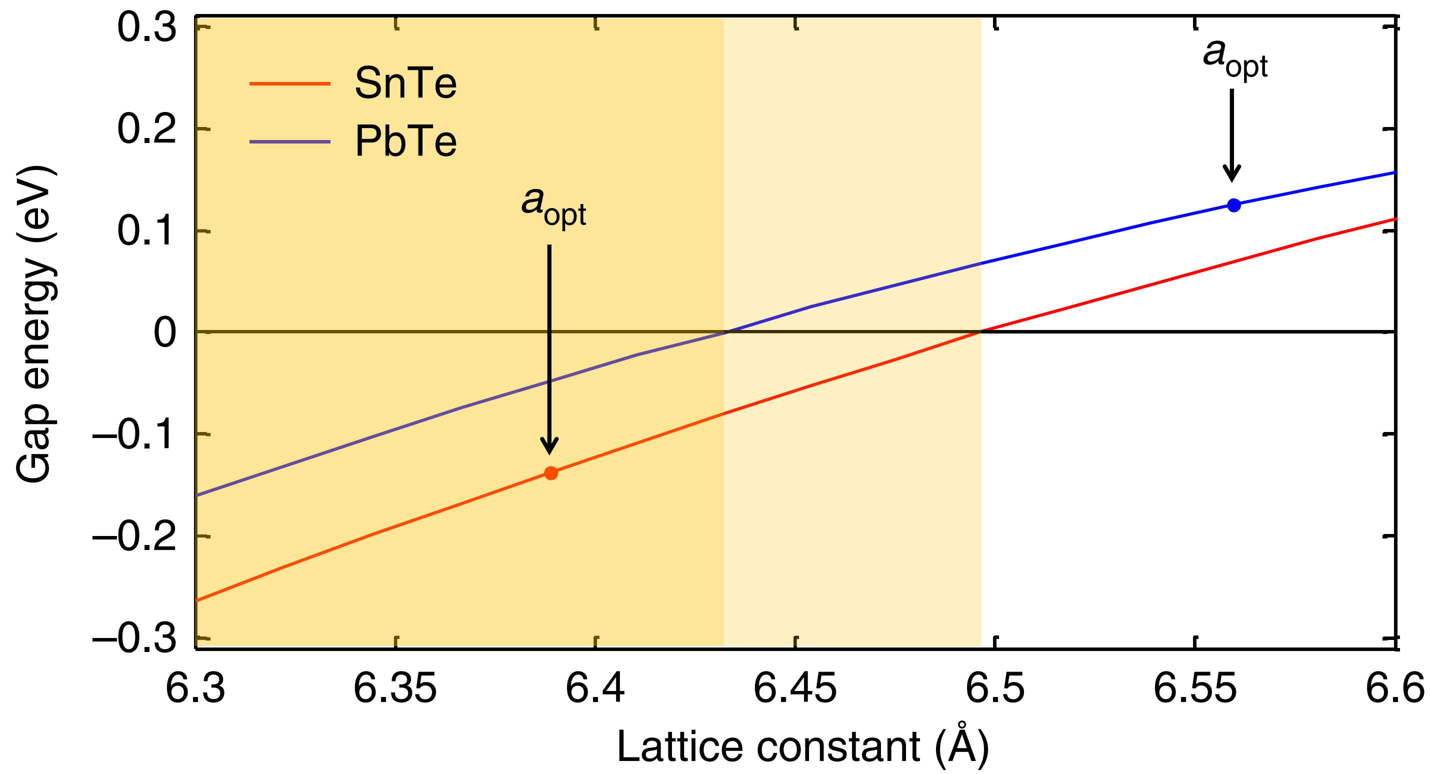
Orbital analysis



- PbTe = ionic insulator $Pb^{2+}Te^{2-}$: trivial
- SnTe is inherently inverted: **topological crystalline insulator**

Inverted Band in SnTe

Band gap vs. lattice constant:



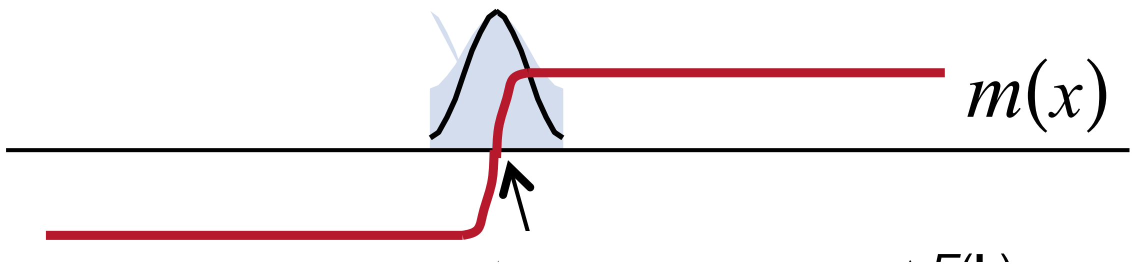
- inverted gap decreases to zero as lattice constant increases:

  agrees with temperature and pressure dependence of band gap in SnTe, but opposite to PbTe

- similar band inversions occur in $Pb_{1-x}Sn_xSe$, and under pressure/strain.

Topological Surface States

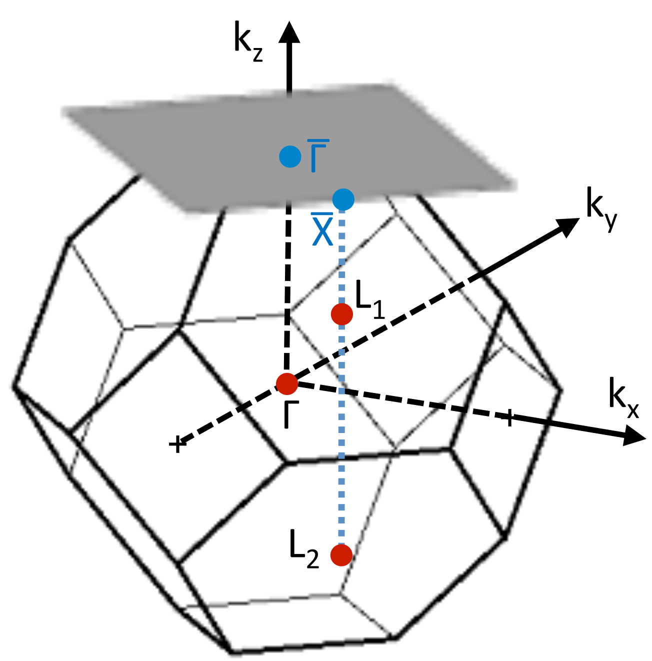
Field-theoretic study of domain wall states: (c.f. Volkov & Pankratov 1985)



treats four valleys independently, misses key effects at lattice scale

2D massless Dirac fermion mass domain all

SnTe (001) surface:

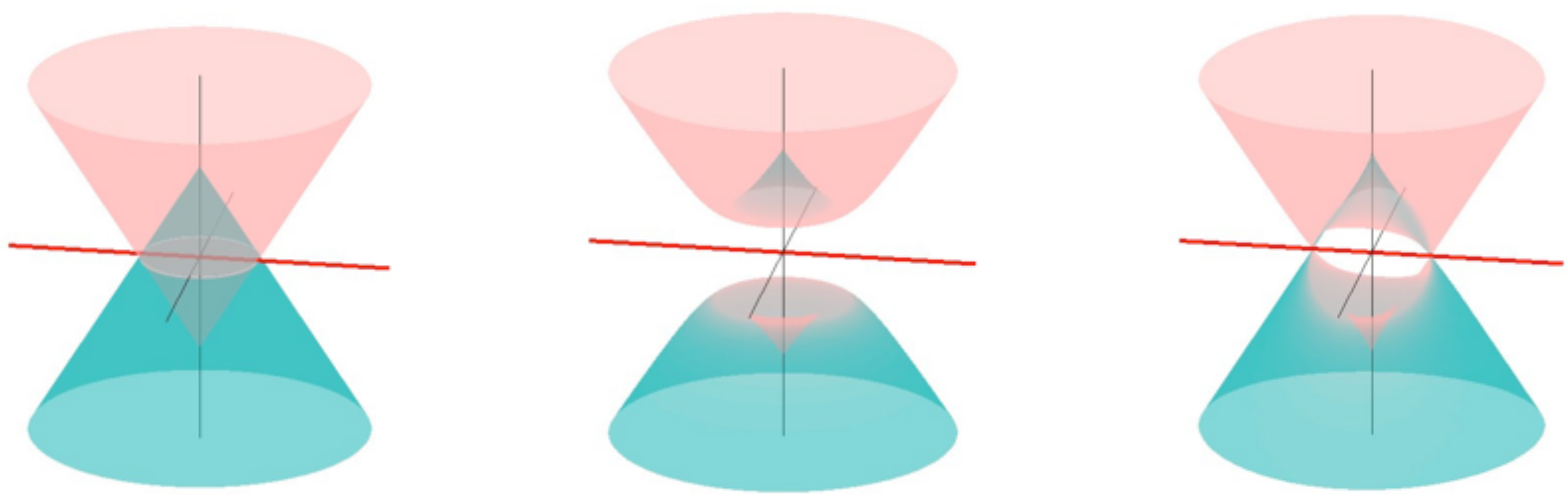


band inversion at both L_1 and L_2

1 “+” 1 = ?

SnTe (001) Surface States

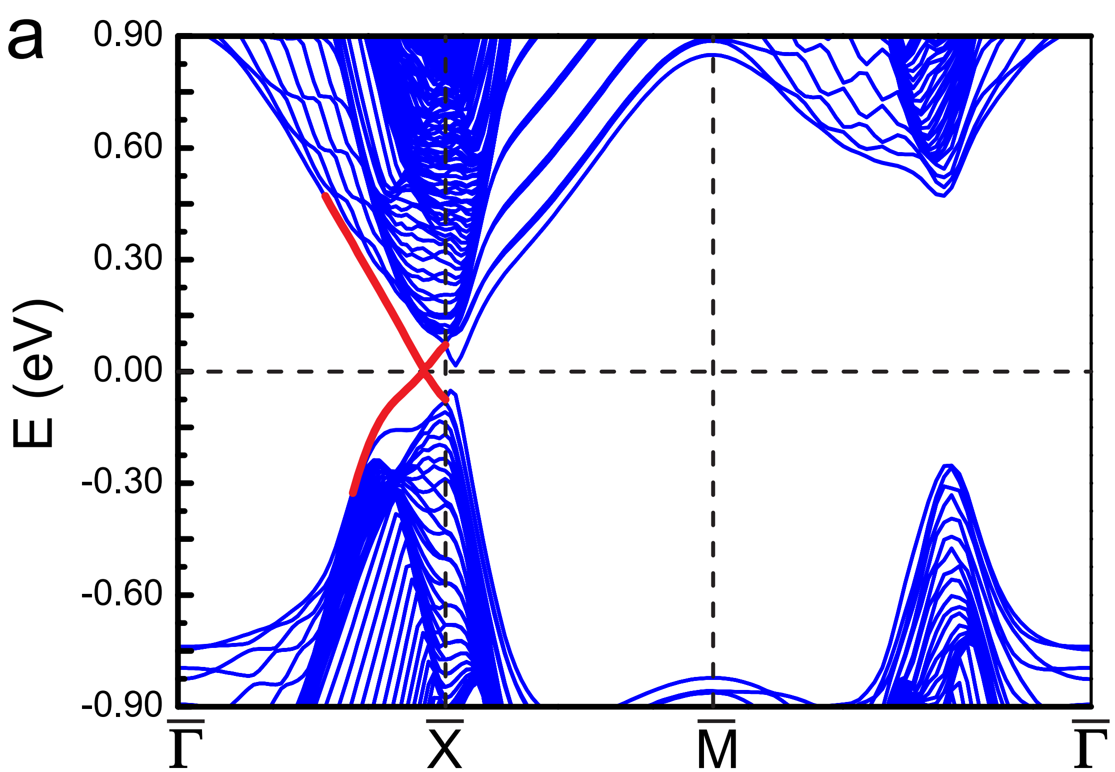
field theory | without symmetry | with mirror symmetry

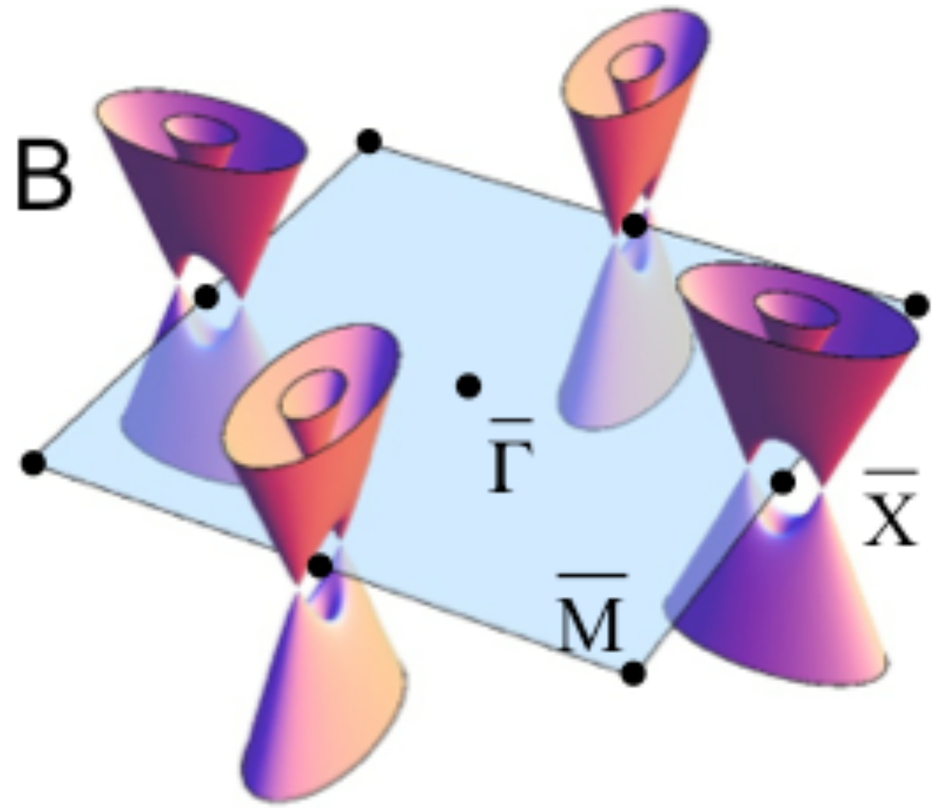


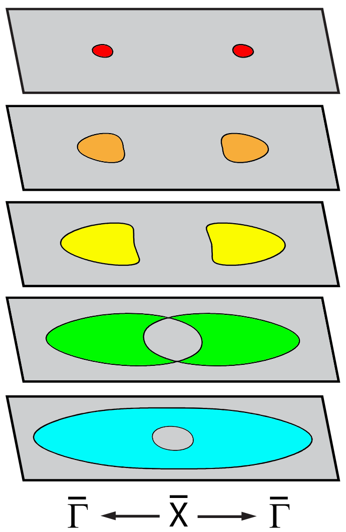
overlapping Dirac fermions | gapped surface | two new Dirac nodes away from X points

- mirror symmetry forbids hybridization along ΓX direction: key to topological crystalline insulator

Prediction: Topological Surface States







001 surface states consist of four Dirac cones located away from X

- spin-momentum locking with same chirality: cannot be realized in 2D
- Fermi surface topology change (**Lifshitz transition**) at higher energy
- Van-Hove singularity: possible interaction-driven phenomena

Experiments

Xu, Hasan et al:

Received 6 Aug 2012 | Accepted 8 Oct 2012 | Published 13 Nov 2012

DOI: 10.1038/ncomms2191

Observation of a topological crystalline insulator phase and topological phase transition in $Pb_{1-x}Sn_xTe$

Tanaka et al:

nature physics

LETTERS

PUBLISHED ONLINE: 30 SEPTEMBER 2012 | DOI: 10.1038/NPHYS2442

Experimental realization of a topological crystalline insulator in SnTe

Dziawa et al:

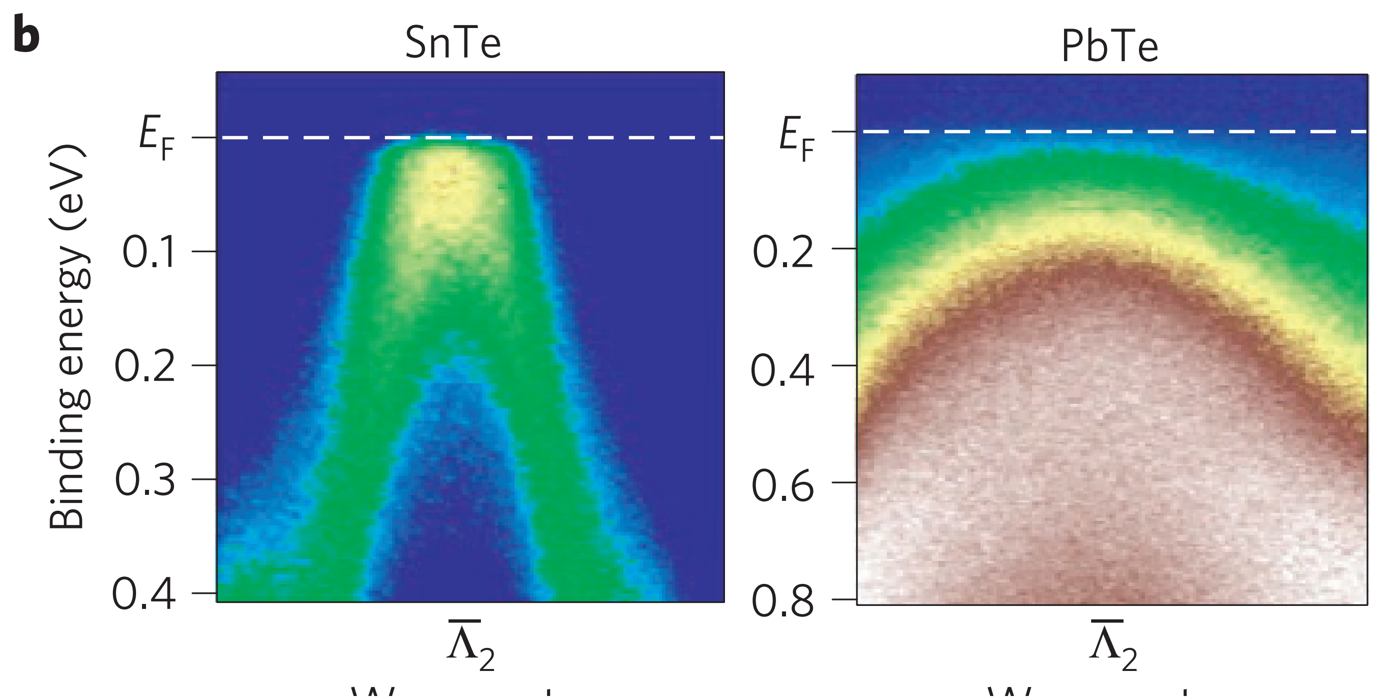
nature materials

LETTERS

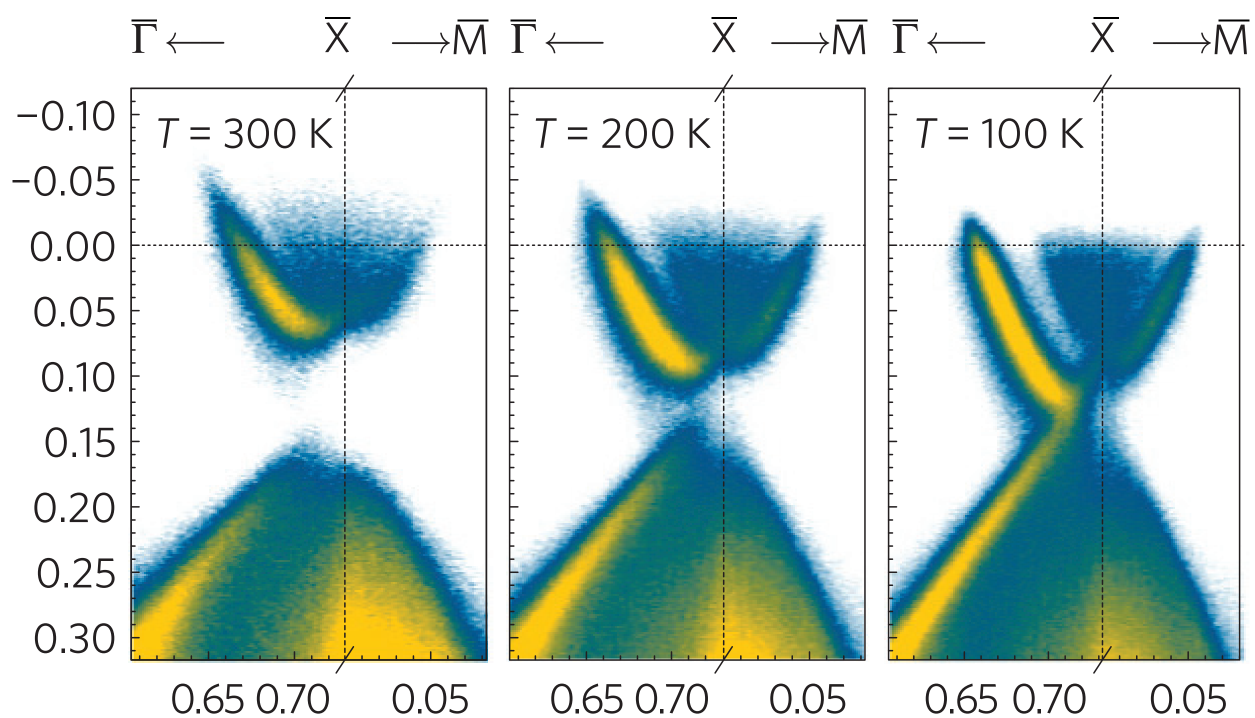
PUBLISHED ONLINE: 30 SEPTEMBER 2012 | DOI: 10.1038/NMAT3449

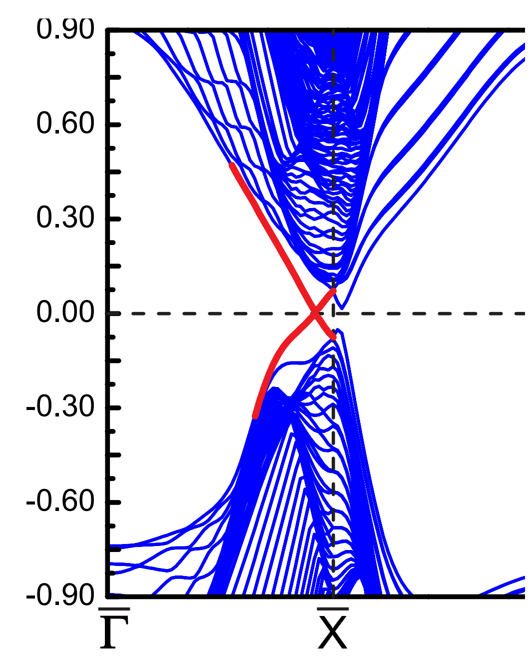
Topological crystalline insulator states in $Pb_{1-x}Sn_xSe$

Tanaka et al: surface states observed in SnTe, but not in PTe

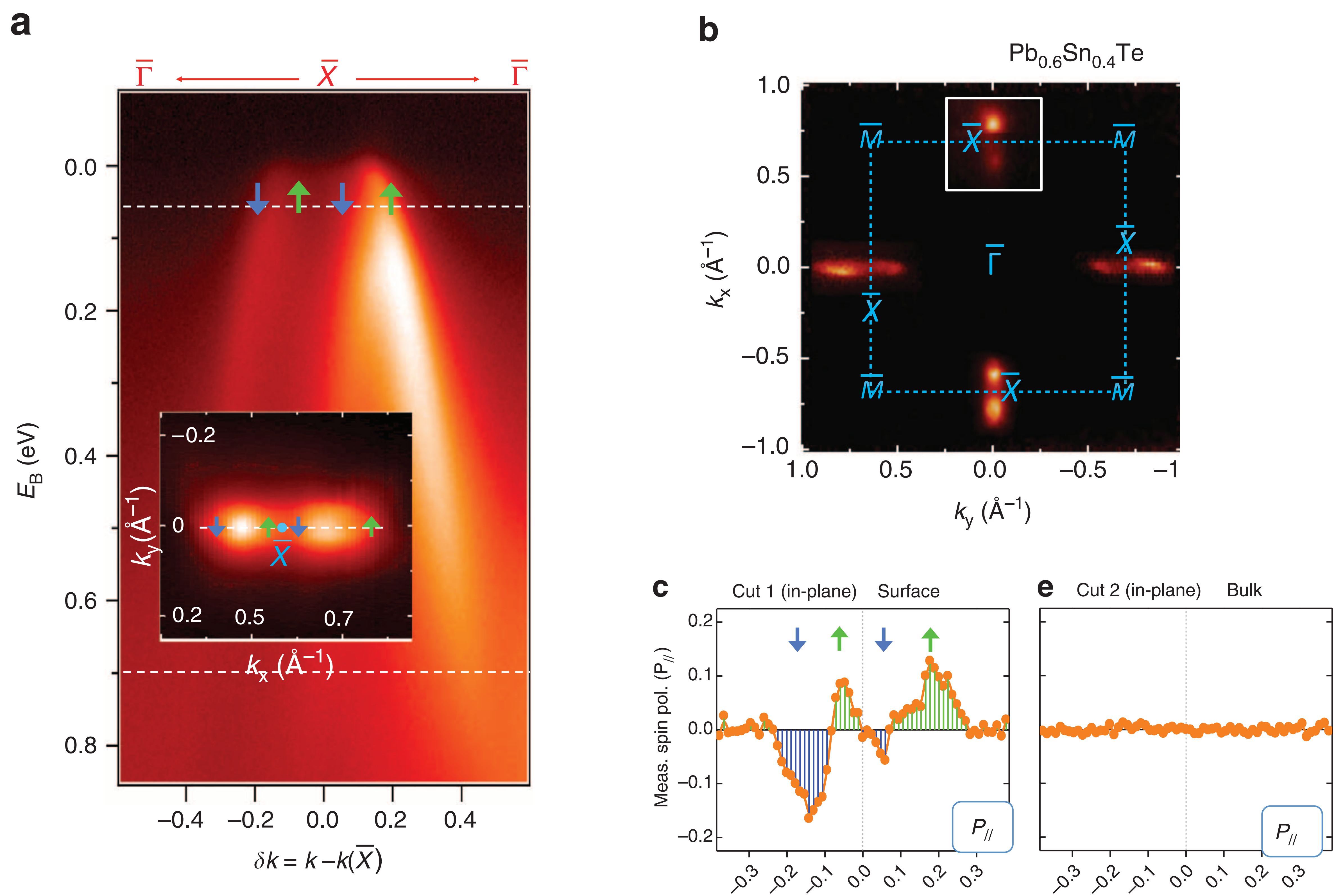


Dziawa et al: temperature driven phase transition in $Pb_{0.77}Sn_{0.23}Se$





Xu et al: spin-resolved measurements



IV-VI Family of Topological Crystalline Insulators

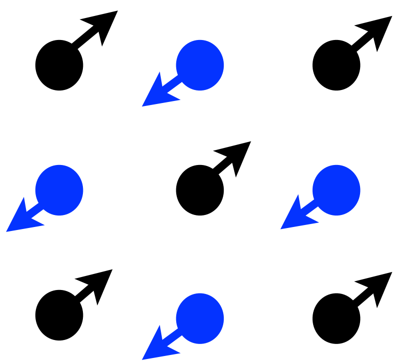
a versatile platform

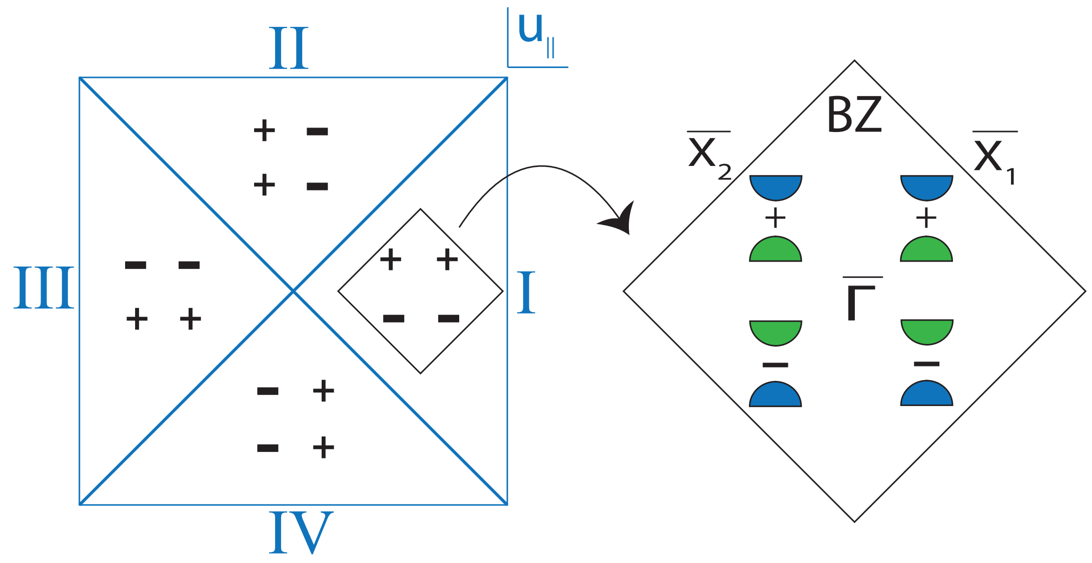
- 3D Dirac material
- very high mobility
- extraordinary tunability by alloying and temperature:
  ferromagnetism, superconductivity, ferroelectricity ...
- thin films and quantum wells
- potential device applications: tunable electronics & spintronics

Ferroelectric Distortion Induces Dirac Gap

Prediction: breaking mirror symmetry generates Dirac mass

ferroelectric displacement





- induced gap depends on direction of in-plane vector u

$$m_j \propto (\mathbf{u} \times \mathbf{K}_j) \cdot \hat{z},$$

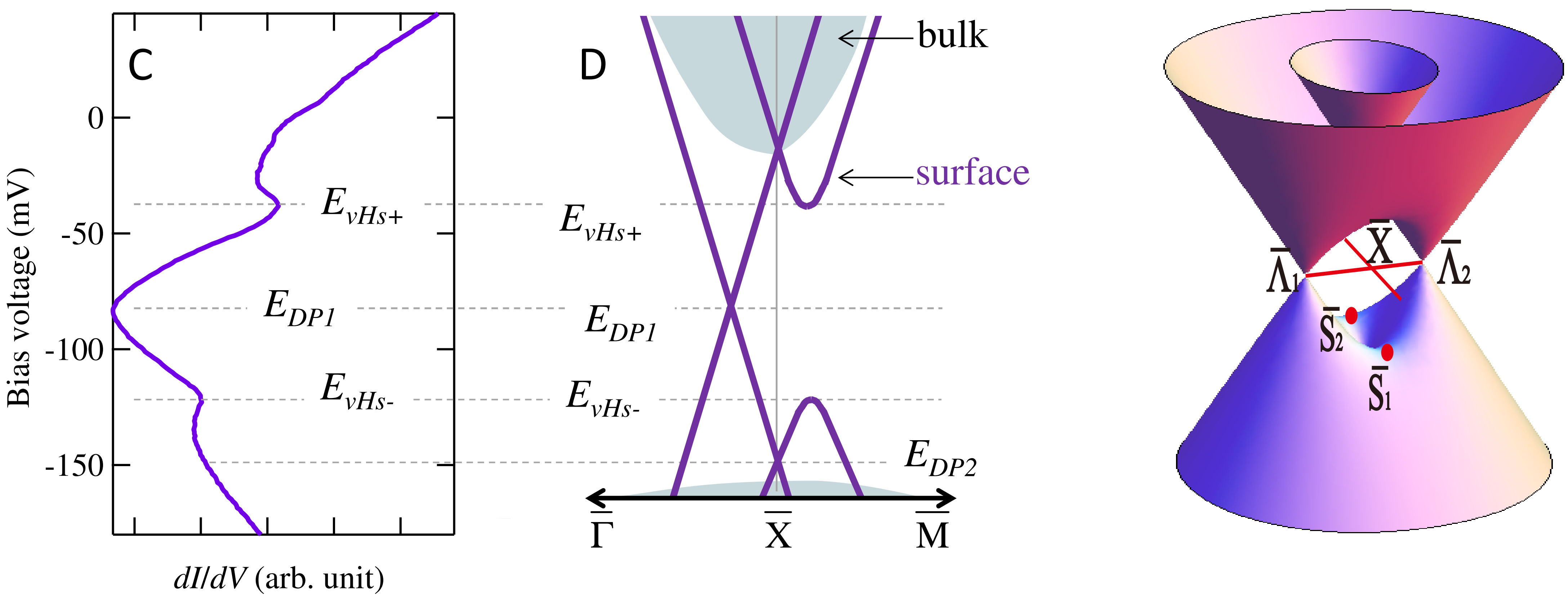
- rhombohedral distortion (known in SnTe) with u along (110):
  breaks one mirror symmetry, but preserves the other

=> two massless Dirac fermions coexist with two massive Dirac fermions

- Dirac masses at k and -k have opposite sign (due to T-symmetry)

Observation of Dirac node formation and mass acquisition in a topological crystalline insulator

Okada, Serbyn et al, arXiv:1305.2823 (submitted to Science)

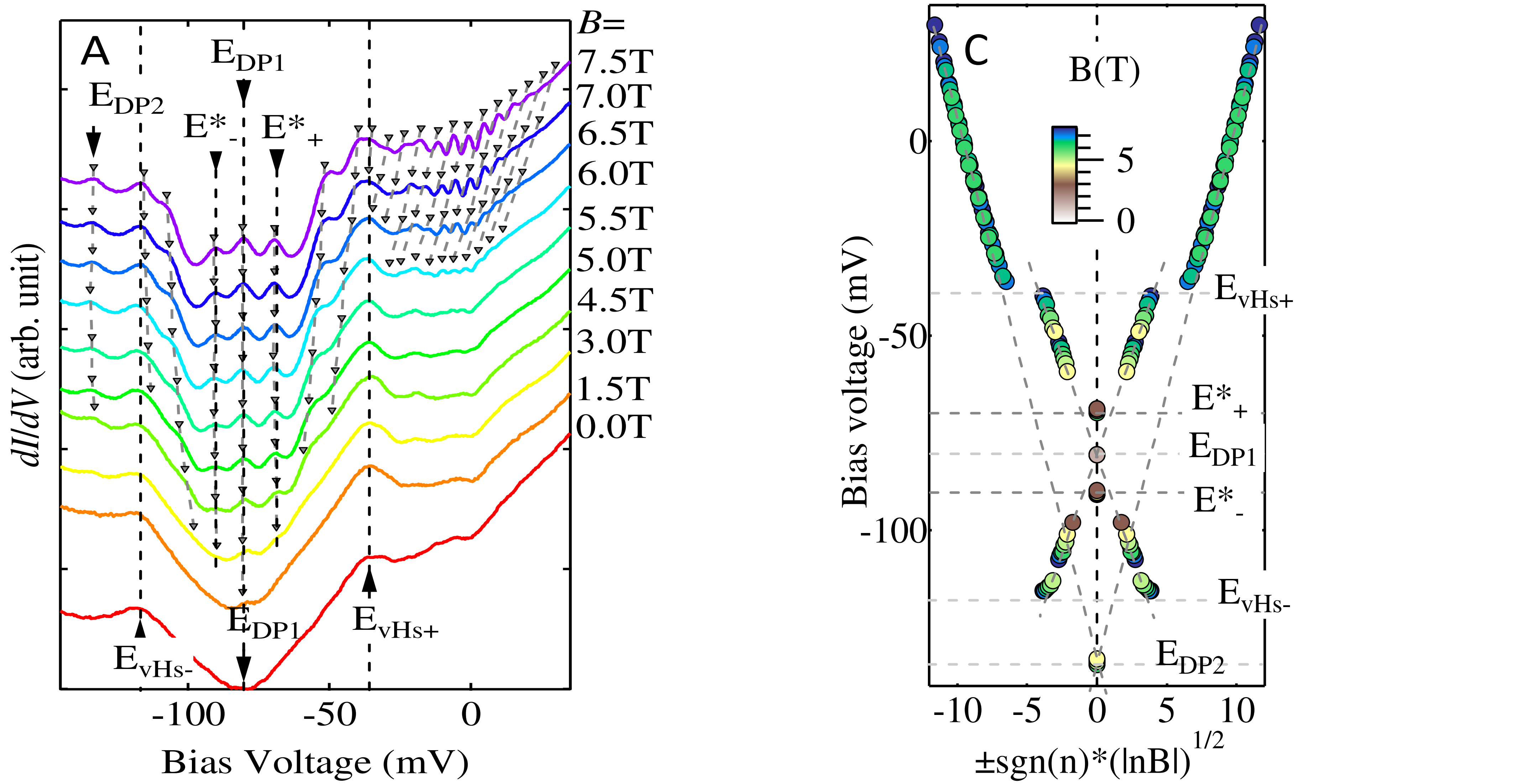


- zero-field dI/dV: linearly dispersing Dirac fermion & Van-Hove singularity

(Liu, Duan & LF, arXiv: 1304.0430)

Observation of Dirac node formation and mass acquisition in a topological crystalline insulator

Okada, Serbyn et al, arXiv:1305.2823 (submitted to Science)



- two non-dispersing Landau levels located symmetrically away from Dirac point
- unique signature of two massive Dirac fermions with opposite masses
- Dirac band gap engineering by strain: topological transistor

Part II. Anderson Transition

Motivation: fate of TCI surface states (in SnTe class) under disorder

- disorder necessarily violates crystal symmetry
- symmetry is restored after disorder averaging
- are TCI surface states robust against strong disorder?

disorder

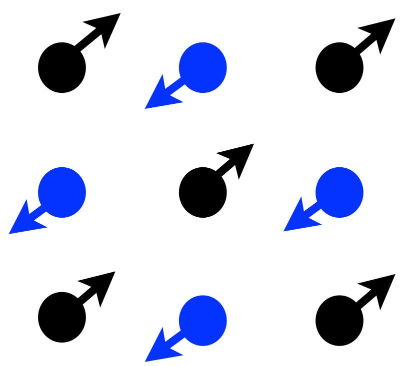
topology
& crystal symmetry

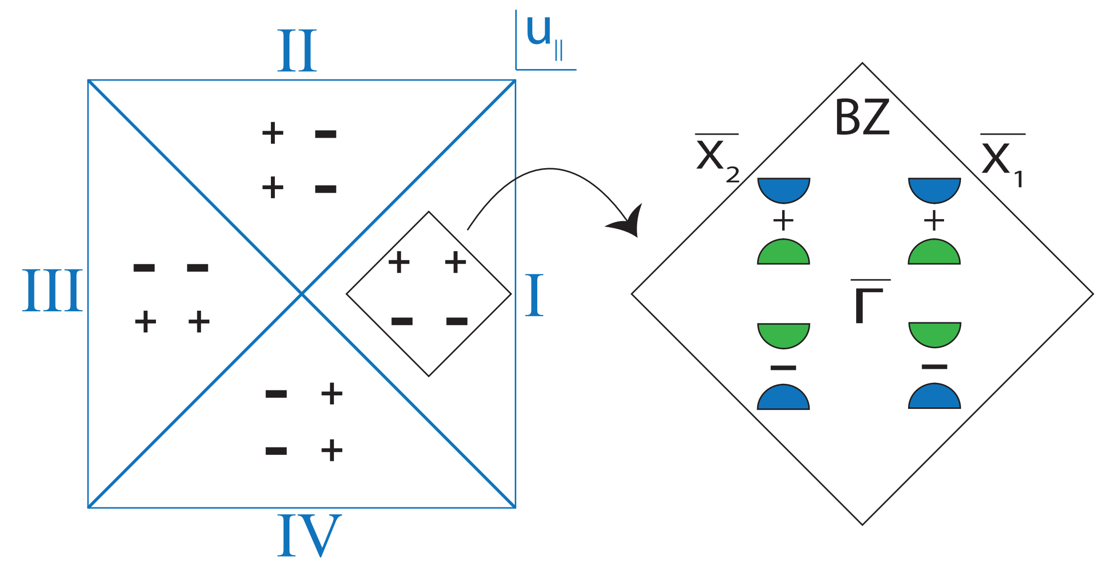
Collaboration with Charlie Kane (UPenn)

Ferroelectricity-induced Gap

Breaking mirror symmetry uniformly generates mass for Dirac surface states:

ferroelectric displacement

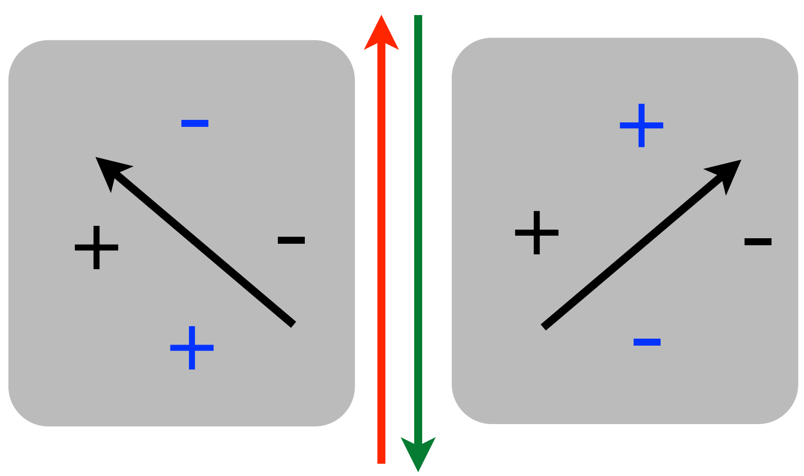




- <u>sign</u> of induced gap depends on direction of u: $m_j \propto (\mathbf{u} \times \mathbf{K}_j) \cdot \hat{z},$

1D helical edge states at domain wall:

- perfect conducting channel w/o backscattering
- detection by STM, AFM



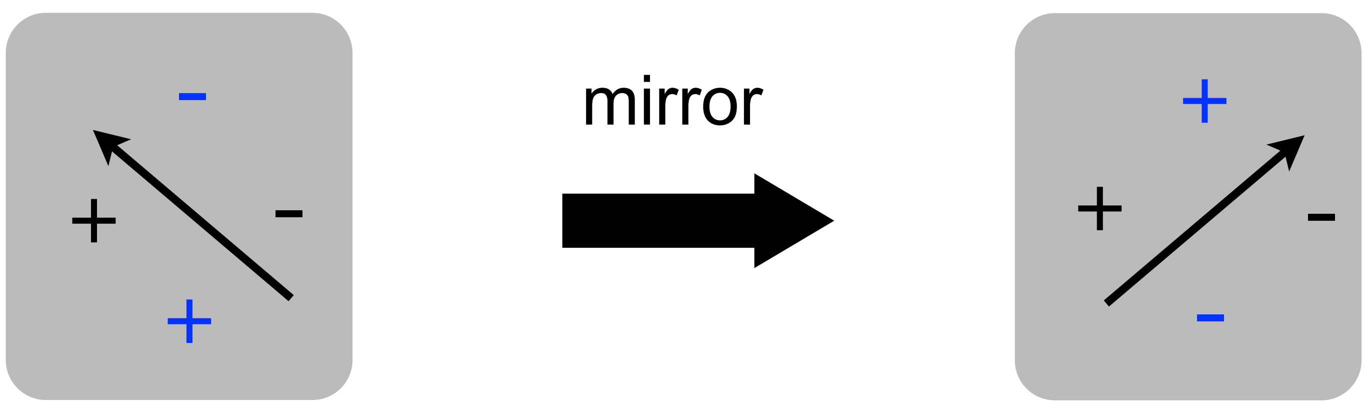
Hsieh, Lin, Liu, Duan, Bansil & LF, Nature Communications, 2012

Anomalous Action of Symmetry on Gapped Boundary

Breaking symmetry leads to a gapped surface with “anomaly”

Topological crystalline insulator:

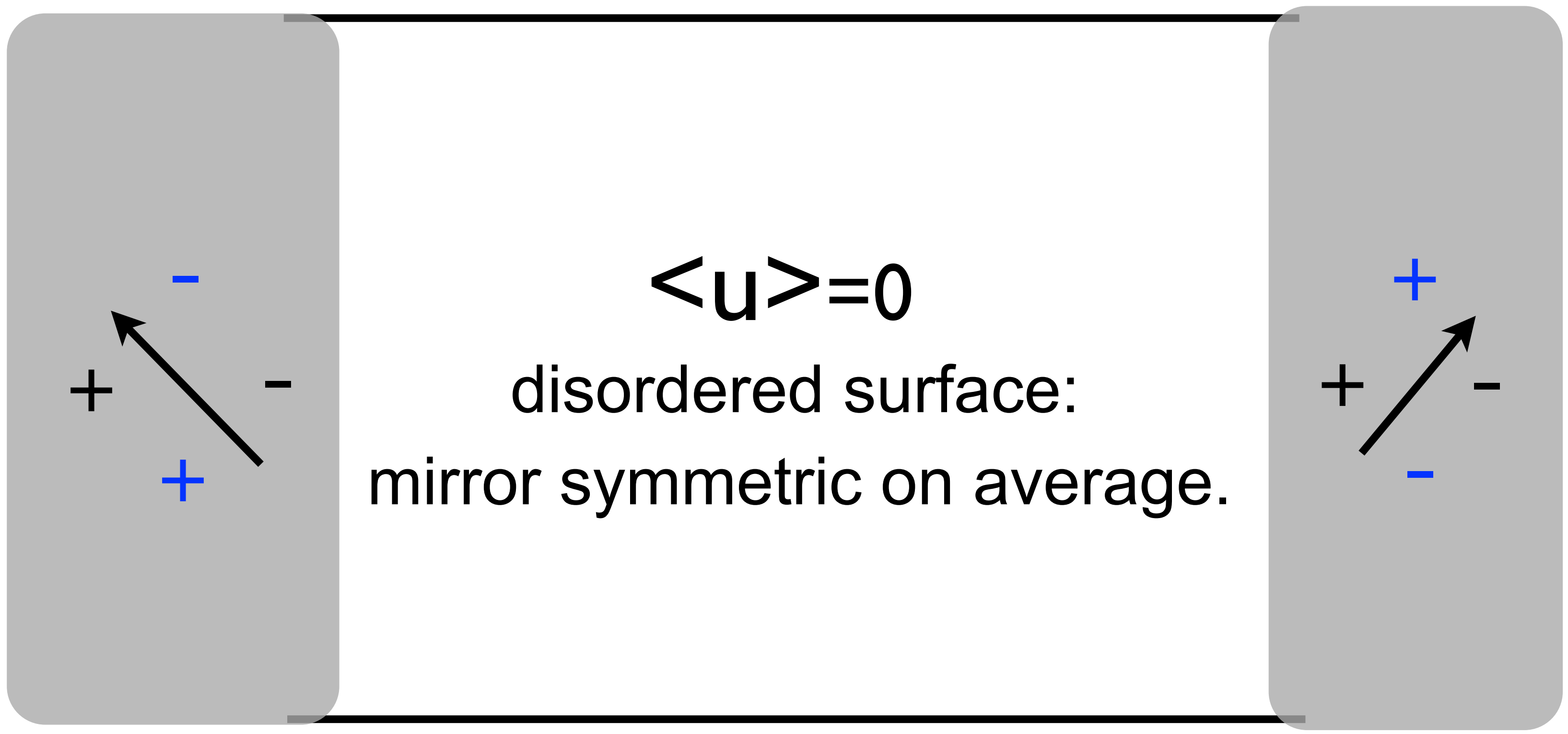
- action of mirror on a gapped surface leads to a state in a different Z_2 class.
- pristine TCI surface is half-way in between two Z_2 distinct states



Topological insulator:

- action of time reversal on a gapped surface changes Hall conductance by one
- pristine TI surface is at a quantum Hall plateau transition

Robustness of TCI Surface States



- If disordered surface were localized, there must be one helical mode localized on either left or right boundary, which would contradict mirror symmetry.

- TCI surface states must remain delocalized even under strong disorder on the surface.

(LF, to appear)

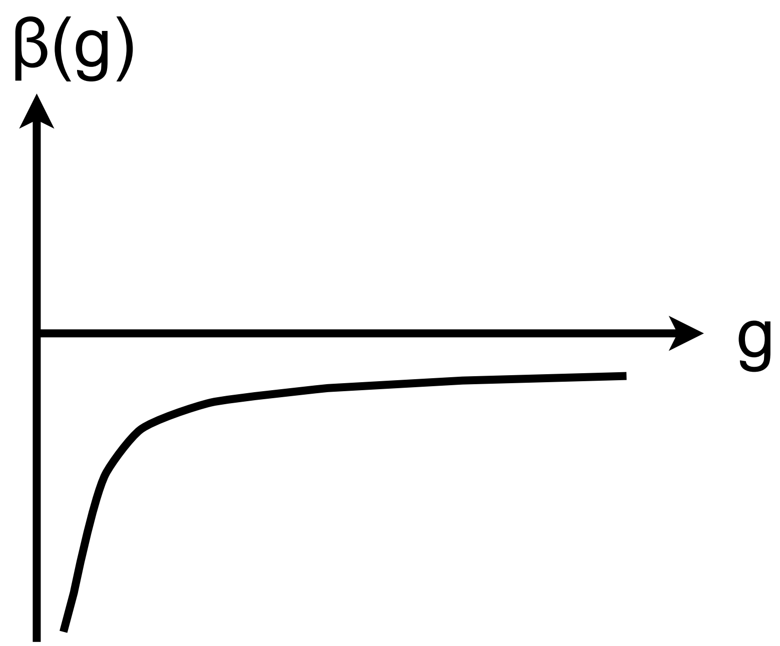
- similar delocalization in weak TI c.f. Ringel, Kraus & Stern, 12; Mong, Bardarson & Moore, 12

Anderson Localization in Two Dimensions

Conventional wisdom:

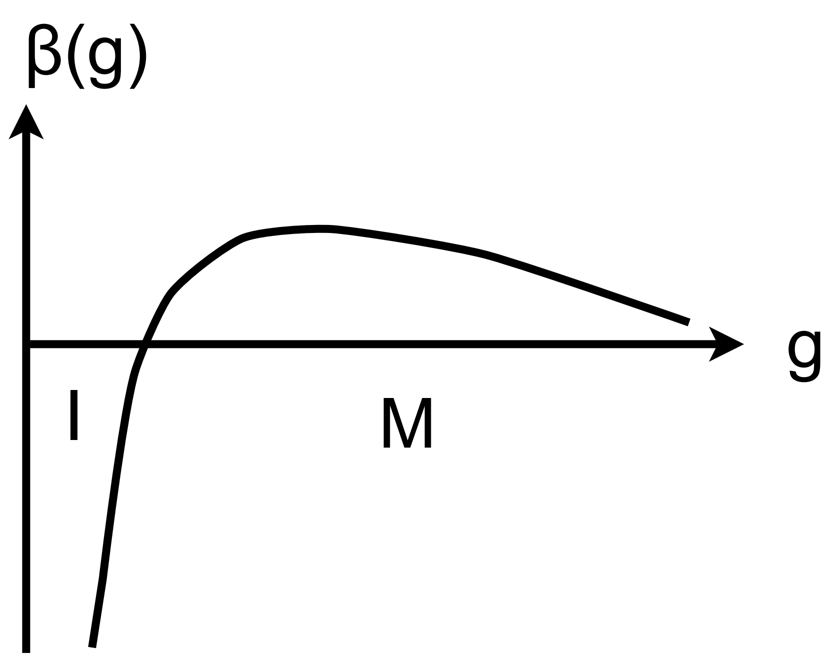
- all states are localized under strong disorder
- one-parameter scaling based on conductance

Orthogonal class
(T-invariant, spinless)



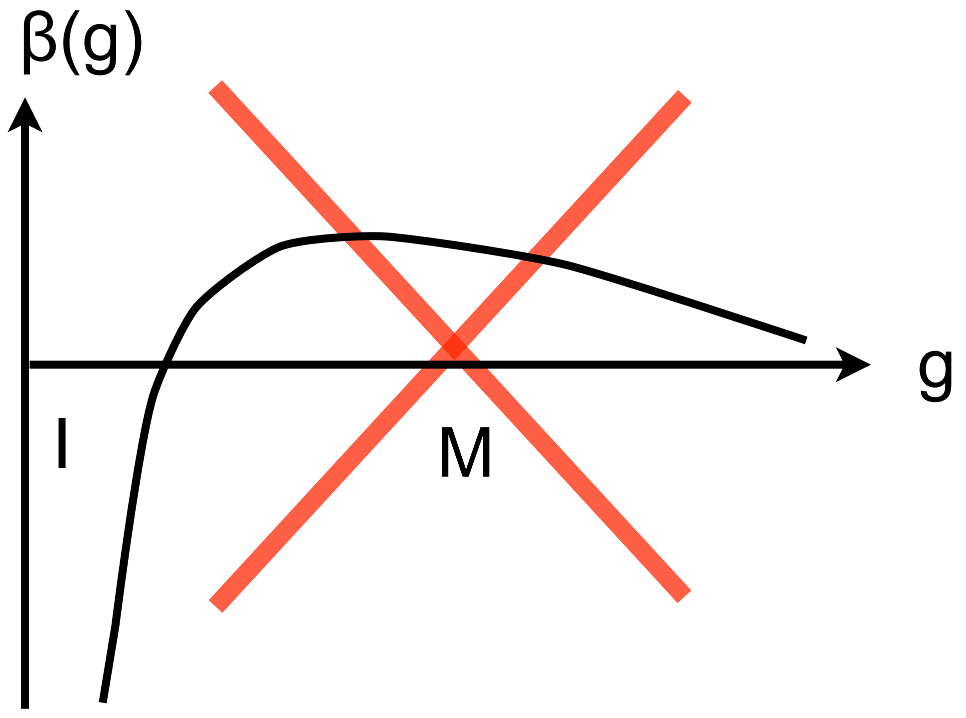
Abrahams, Anderson, Liccoardello
& Ramakrishnan, 1979

Symplectic class
(T-invariant, spin-orbit)



Hikami, Larkin, Nagaoka, 1980

Anderson Transition in Symplectic Class



Single-parameter scaling theory is wrong, because

- it does not distinguish two localized phases: trivial & 2D TI
- it cannot explain absence of localization under strong disorder on TCI

Field Theory

Nonlinear sigma model in replica limit N=0

$$S_0[Q] = \frac{1}{32\pi t}\int d^2r \mathrm{Tr}[(\nabla Q)^2] \qquad Z = \sum_Q e^{-S_0[Q]}$$

$Q \in O(2N)/O(N) \times O(N)$ is order parameter for metal-insulator transition

Topological Defects in Field Theory

Nonlinear sigma model in replica limit N=0

$$S_0[Q] = \frac{1}{32\pi t}\int d^2r \mathrm{Tr}[(\nabla Q)^2] \qquad Z = \sum_Q v^{N_{\mathrm{vortex}}[Q]} e^{-S_0[Q]}$$

$Q \in O(2N)/O(N)\times O(N)$ is order parameter for metal-insulator transition

New ingredient: vortices in NLsM $\pi_1(O(2N)/O(N)\times O(N)) = Z_2$

To determine vortex fugacity v:

integrate out Grassman variables in the presence of a vortex

$$e^{-S_{\mathrm{eff}}[Q]} = \int D[\bar{\psi},\psi] e^{-\int d^2r[\bar{\psi}_a[(\mathcal{H}_0 - E)\delta_{ab} + i\Delta Q_{ab}]\psi_b]}$$

v is given by Pfaffian of kernel: $v = \frac{\mathrm{Pf}[i\sigma^y D(Q)]}{\mathrm{Pf}[i\sigma^y D(Q_0)]},$

LF & Kane, PRL 109, 246605 (2012).

Vortex Fugacity: a Sign of Topology

Consider a 2D system near the transition between trivial and topological:

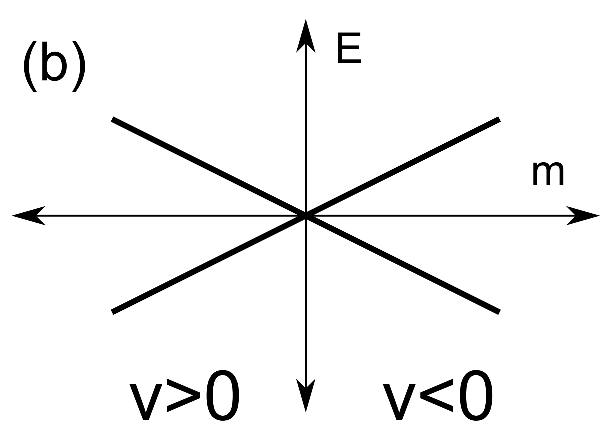
$$H_0 = v_x \sigma_x k_x + v_y \sigma_y \tau_z k_y + m \sigma_y \tau_y$$

- m<0 and m>0 are distinct gapped phases
- m=0 for surface of TCI, protected by mirror symmetry

Vortex configuration of Q: $$Q(\theta) = 1_{N-1} \oplus \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \oplus 1_{N-1}.$$

Evaluate Pfaffian: Pf = $\prod_i \sqrt{\xi_i}$

- spectrum is particle-hole symmetric
- level crossing in vortex core as m changes sign



Vortex fugacity v characterizes different phases:

v>0 for trivial insulator, v<0 for 2D topological insulator

v=0 at the transition, or for surface of TCI

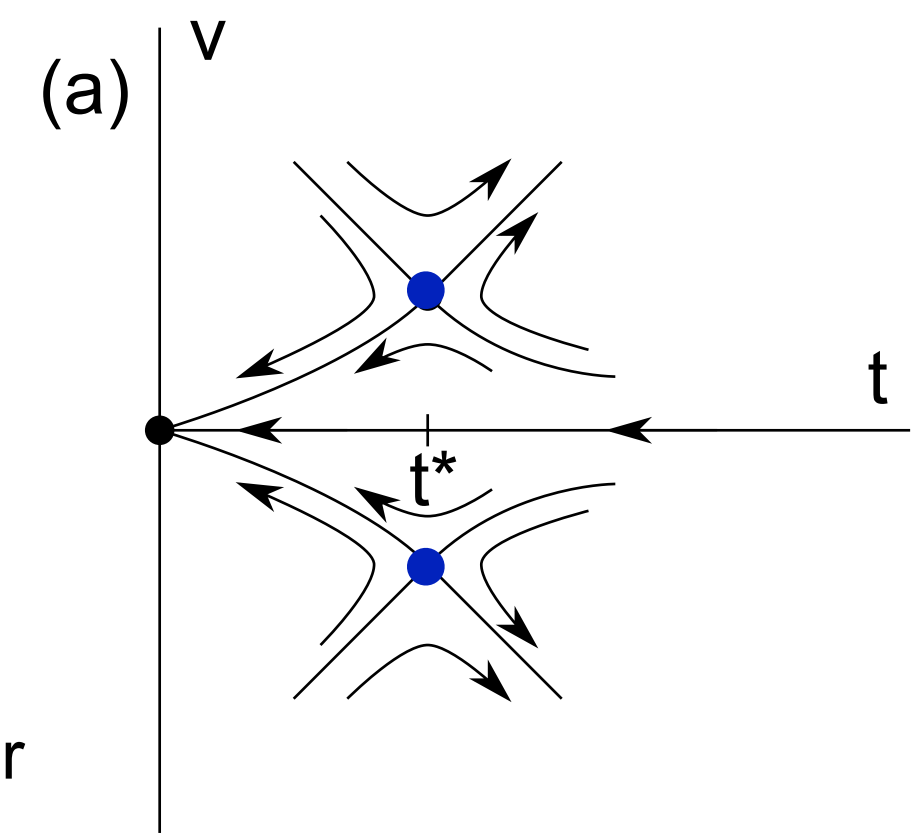
Two-Parameter Scaling Theory

N=1: xy model $$S_{N=1} = \frac{1}{16\pi t} \int d^2 r (\nabla\theta)^2.$$

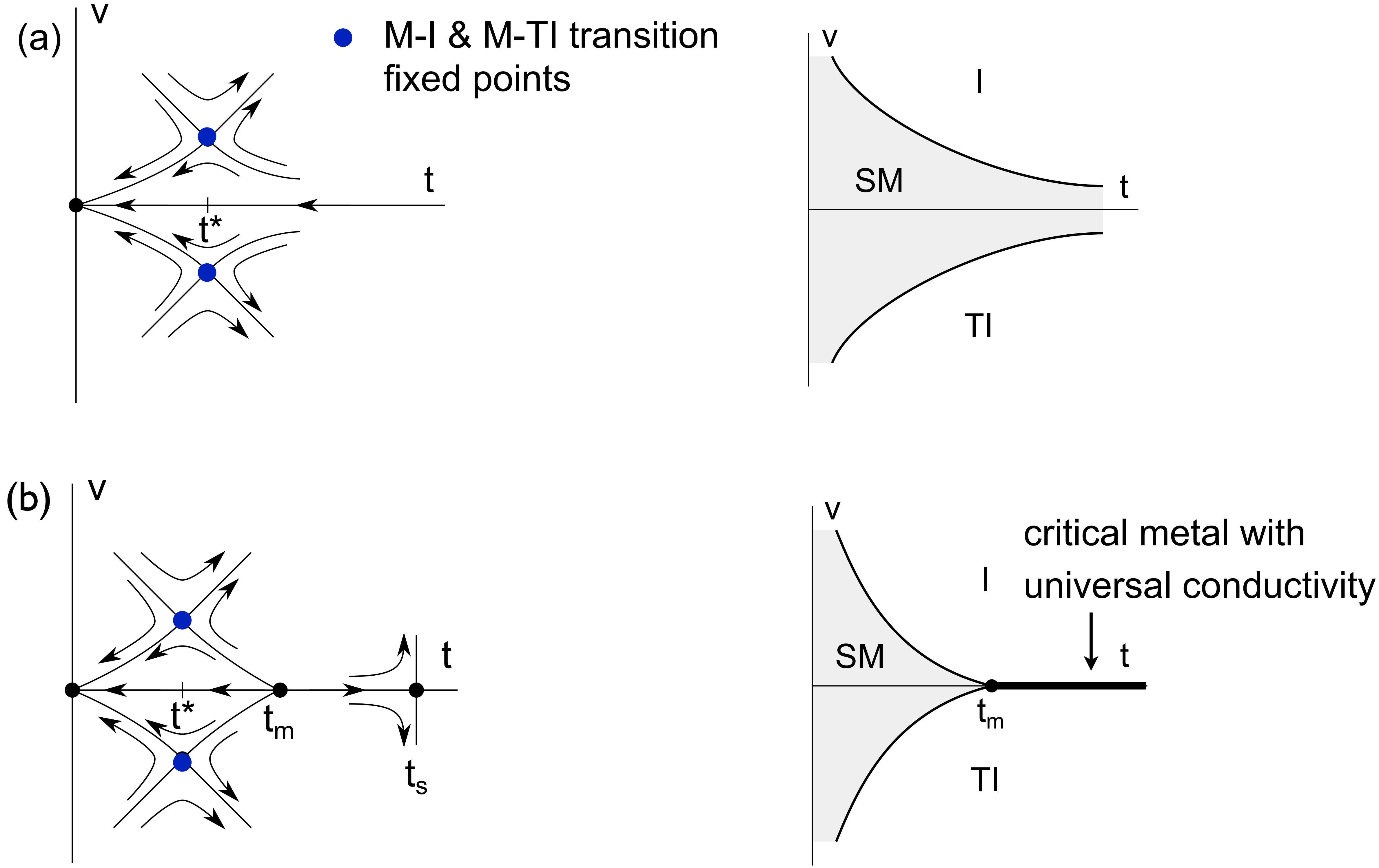
- β(t) = 0
- vortices become relevant at t=1/16 (KT transition)

N=1-ε: ε expansion towards replica limit (ε=1)

$$\begin{aligned} dt/d\ell &= -\epsilon\tilde{\beta}(t) + v^2 \quad \tilde{\beta}(t) = t^2 + \ldots \\ dv/d\ell &= (2 - (8t)^{-1})v. \end{aligned}$$



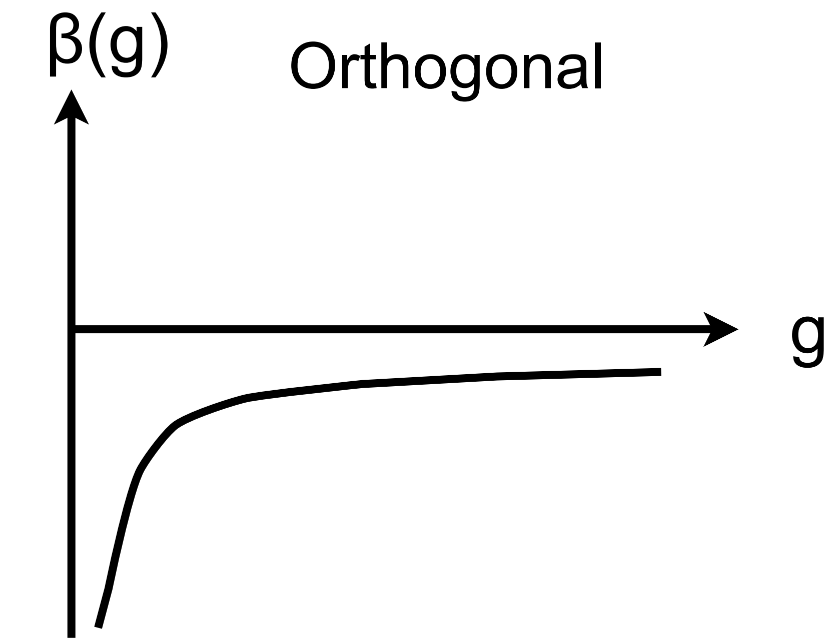
- small t, v flows to 0: symplectic metal
- two new fixed points at v≠0:
  transition from metal to trivial/topological insulator



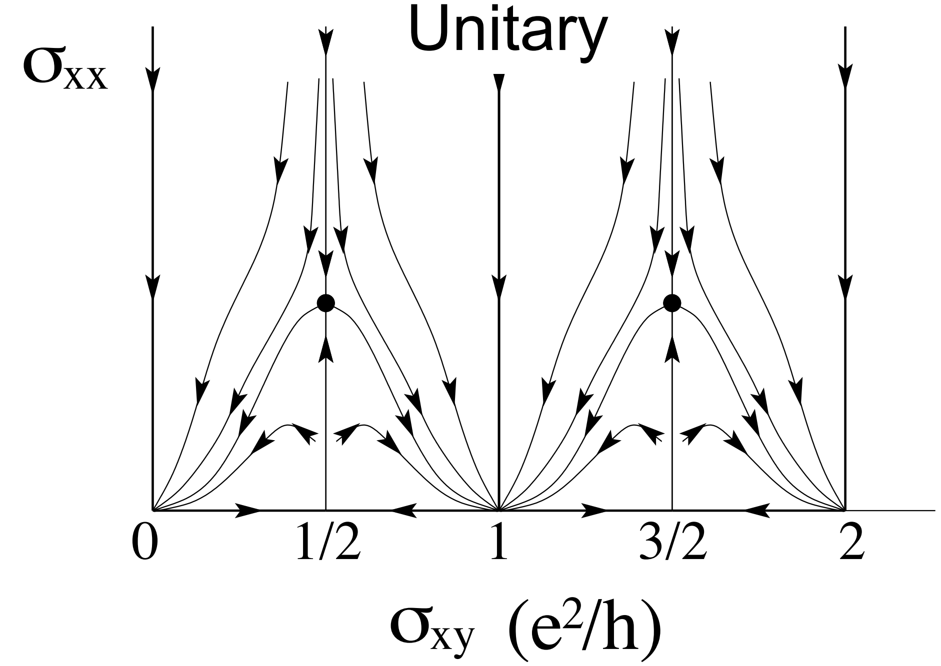
Delocalization of TCI surface states implies:

- vortex proliferation is the sole mechanism of localization
- NLsM in the replica limit cannot be disordered at v=0.

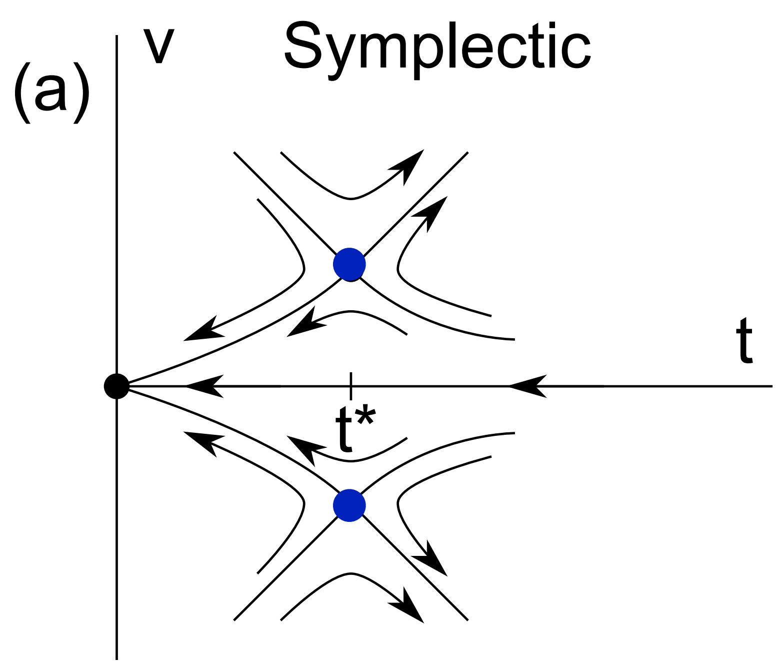
Anderson Localization v.s. Anderson Transition



- all states are localized

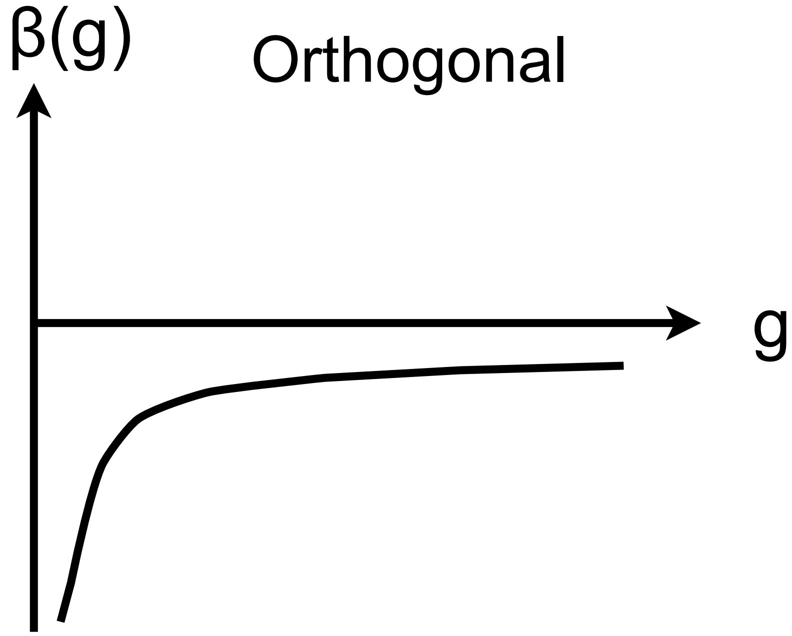


- delocalization at criticality

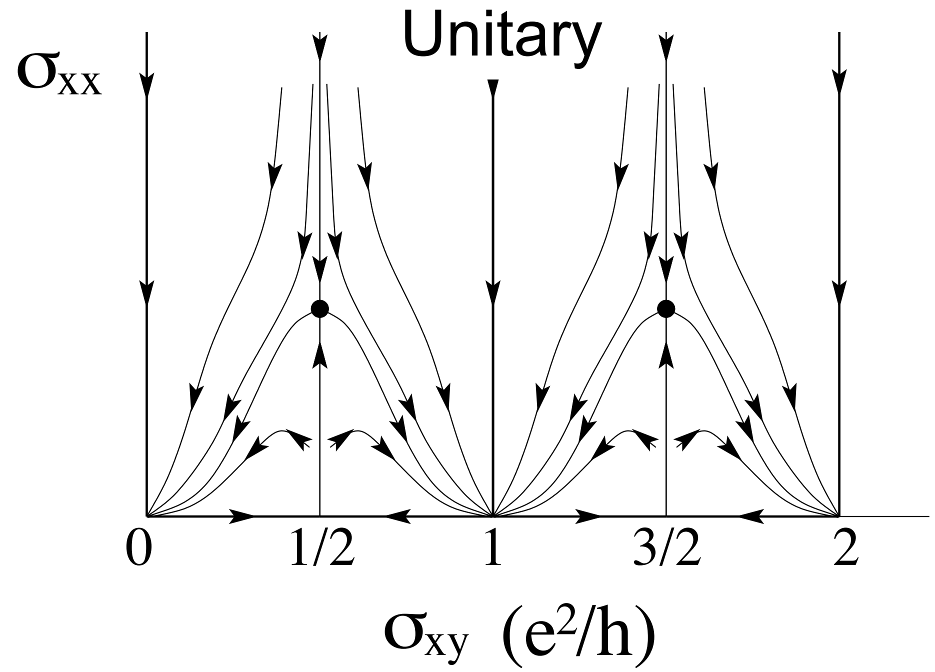


- metal-insulator transition

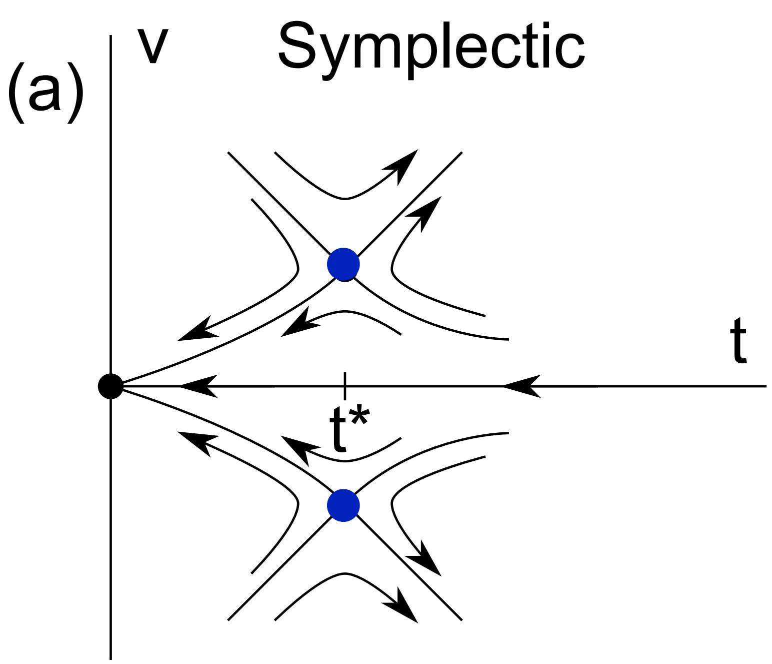
Anderson Localization v.s. Anderson Transition



- all states are localized



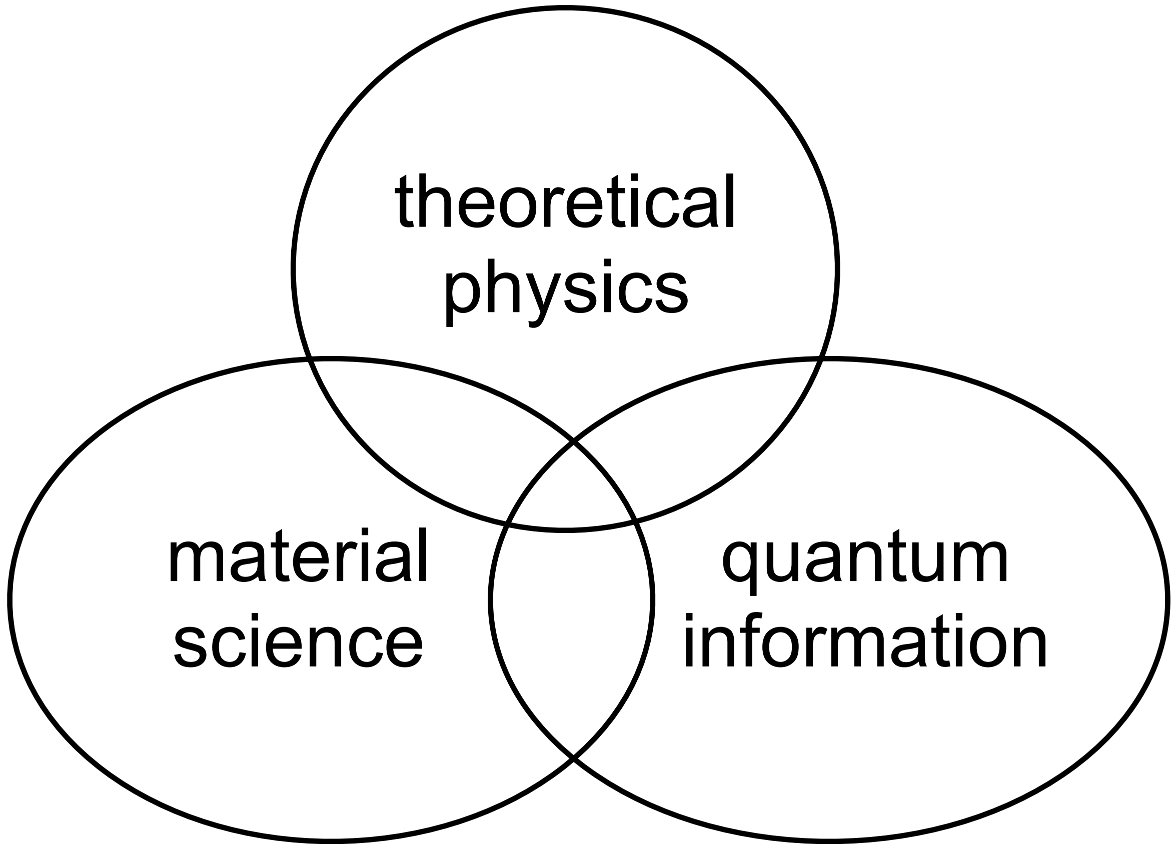
- delocalization at criticality



- metal-insulator transition

topological phase transition

Topological Materials



Thank you !