Metallic Topological Defects inside a Topological Band Insulator

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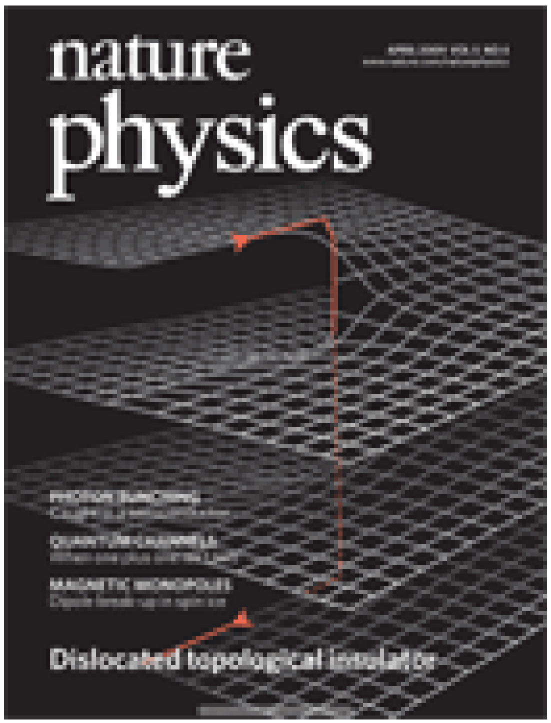


Ying Ran
(UCB=> B.U.)

Yi Zhang

Ref: Nature Physics 5, 289 (2009).
arXiv:0810.5121

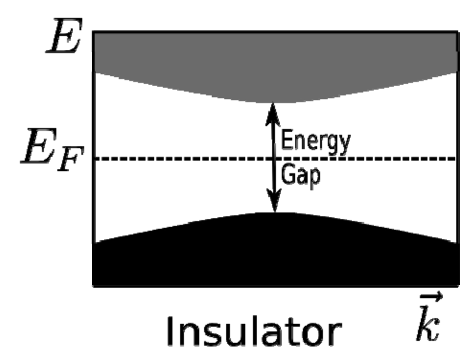
What is topological band insulator?

- Topology characterizes the identity of objects up to deformation, e.g. genus of surfaces

Figure courtesy C. Kane

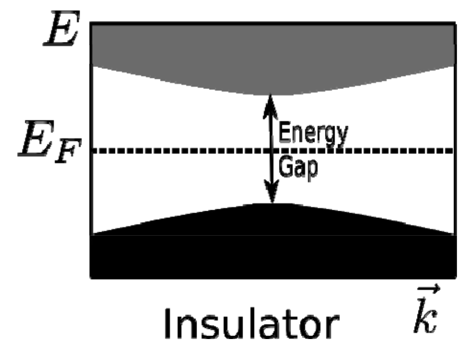
- Similarly, band insulator can be classified up to the deformation of band structure. Modify H smoothly preserving gap.

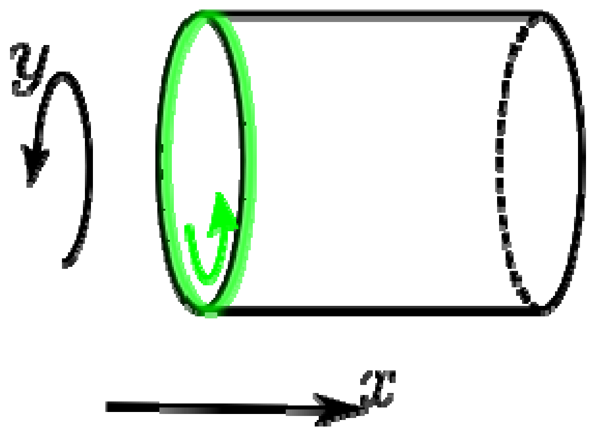
Simplest example- quantum hall insulator.

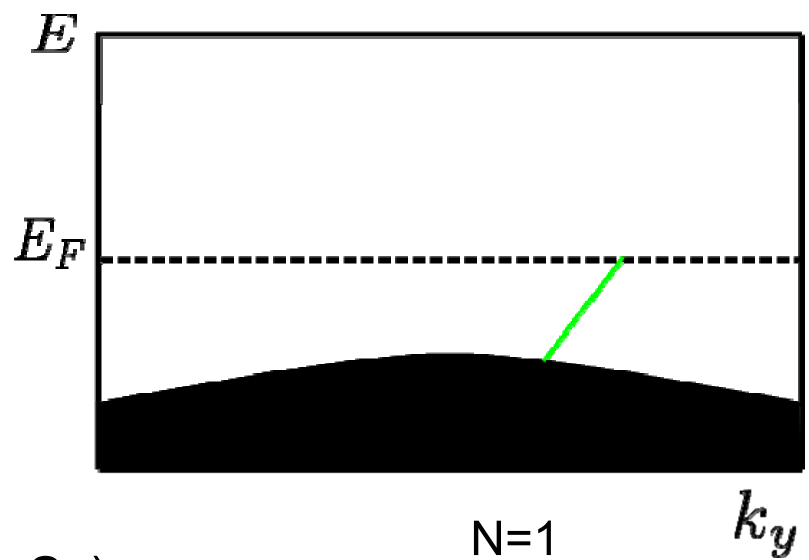


Exotic Band Topology

- Integer Quantum Hall States:
  - Gapped in the bulk
  - Gapless Edge states that are **chiral**
    - (propagate in one direction only)
  - Leads to Quantized Hall effect







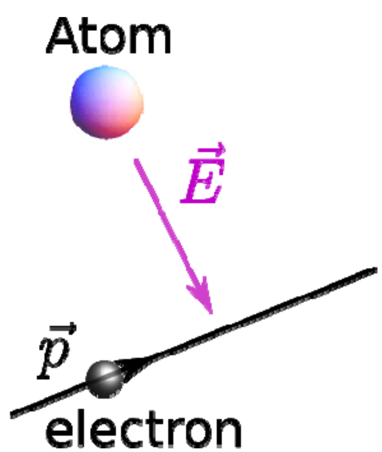
Also, superconducting analogs (p+ip Sc)

Unconventional Surface/Edge states.

"The edge is the window into the bulk" – X.G. Wen

Can one realize a quantum hall like insulator WITHOUT a magnetic field?

- Yes: Kane and Mele; Bernevig & Zhang (2005),
  - Spin-orbit interaction » spin-dependent magnetic field



$$H_{SO} = -\vec{\mu}_{spin} \cdot \left(-\frac{\vec{v} \times \vec{E}}{c^2} \right) \propto \vec{S} \cdot \vec{L}$$

$\updownarrow$

Spin-orbit interaction is Time Reversal symmetric:

$\vec{B}$ for $\uparrow$, $-\vec{B}$ for $\downarrow$.

⇩

"Spin-Hall Effect"

Topological insulator with spin-orbit interaction in D=2

- in 2D, with spin-orbit interaction, time-reversal symmetric topological insulator is labeled by a Z_2 number ν,

ν=0: trivial; ν=1: non-trivial

New phase of matter! (necessarily separated from trivial case by phase transition)

C. Kane

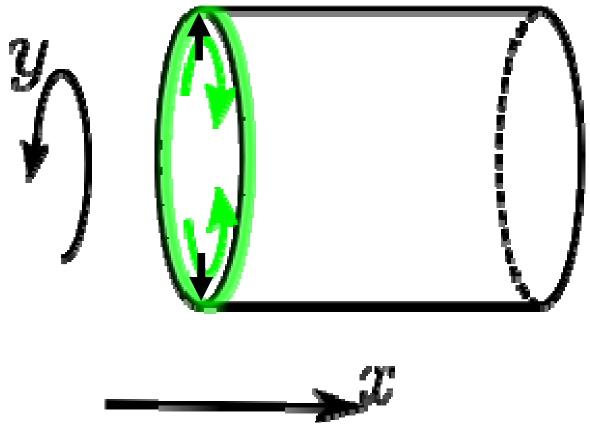
E. J. Mele

Quantum Spin Hall Insulator
or
2D topological Insulator

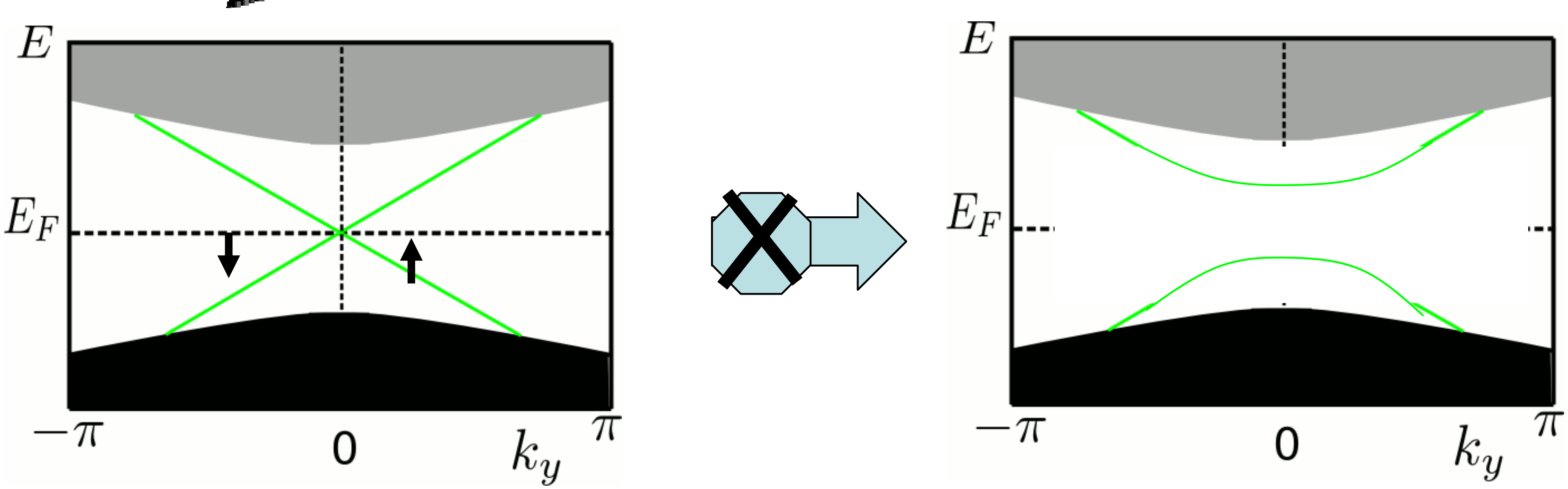
What are the edge states?

Edge states of TR symmetric Z_2 T-I

Time reversal symmetry =>two counter-propagating edge modes



Protected by Time Reversal,
even if spin is not conserved.
Only Z_2 (even-odd) distinction.

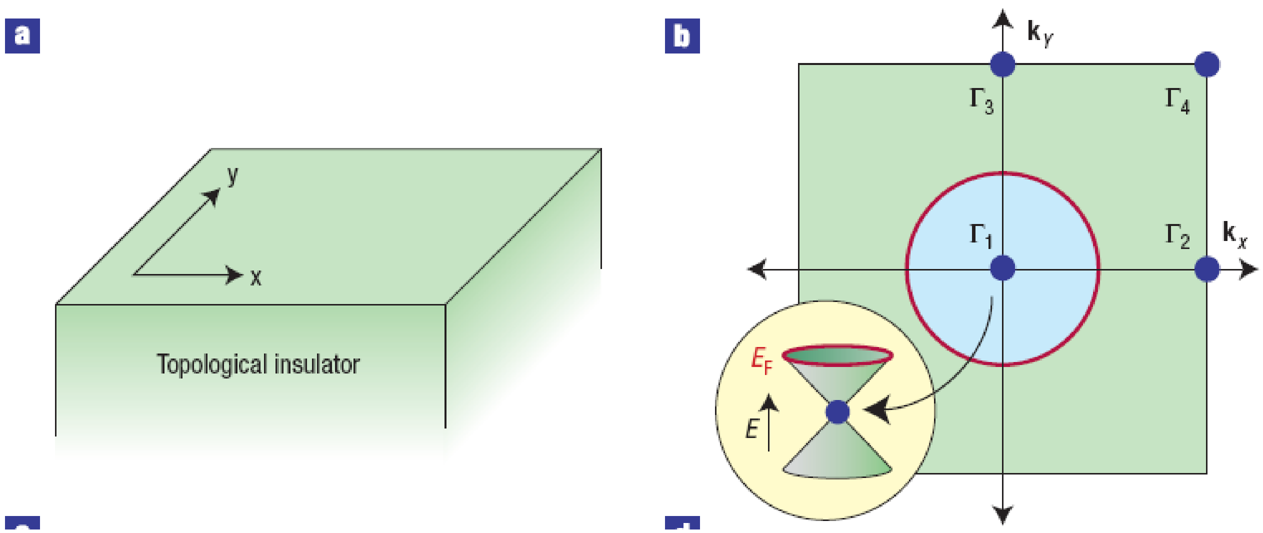


•Experimentally observed by transport measurements on HgTe quantum well (Bernevig et al., Science 2006; Konig etal. Science 2007)

Topological insulator with spin-orbit interaction in D=3

- One obvious route to topological insulator in D=3 :
  - Stack 2D layers of quantum spin Hall insulators.
  - Defined by the reciprocal vector of the stacking layers. $\mathbf{G}_\nu$
  - 'weak' topological insulators.
- Less obvious possibility (no quantum Hall analog)
  - 'strong' topological insulators in D=3.
  - Characteristic feature – Surface state: single Dirac node.

Fu, Kane & Mele (2006), Moore & Balents (2006), Roy (2006).

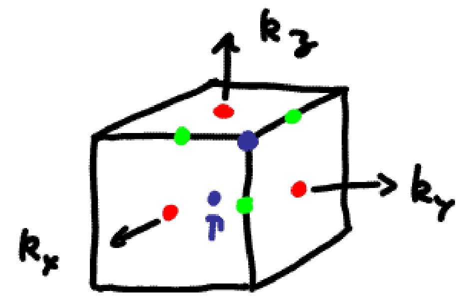


Topological Indices in 3D

- Given a band structure, it is possible to calculate the following topological indices:

Strong index $\nu_0 \in (0,1)$:

Physical Interpretation: ν_0=1=>Odd number of surface Dirac nodes



'Weak' or Lattice indices: $\mathbf{M}_\nu$

time rev. invariant wave-vector $\mathbf{M}_\nu = \frac{1}{2}\mathbf{G}_\nu$

$$\mathbf{M}_\nu = (\nu_1 \mathbf{G}_1 + \nu_2 \mathbf{G}_2 + \nu_3 \mathbf{G}_3)/2$$

Physical Interpretation:

For Strong Insulator:

Location of Dirac node on Surface B.Zone (project $\mathbf{M}_\nu$ on surface)

For Weak insulator:

Stacking of 2D quantum spin Hall layers $\mathbf{M}_\nu = \mathbf{G}_\nu / 2$

OR Location of one of the pair of Dirac nodes on surface (other at Γ)

ν_0 =0 AND $\mathbf{M}_\nu = 0$: then trivial insulator

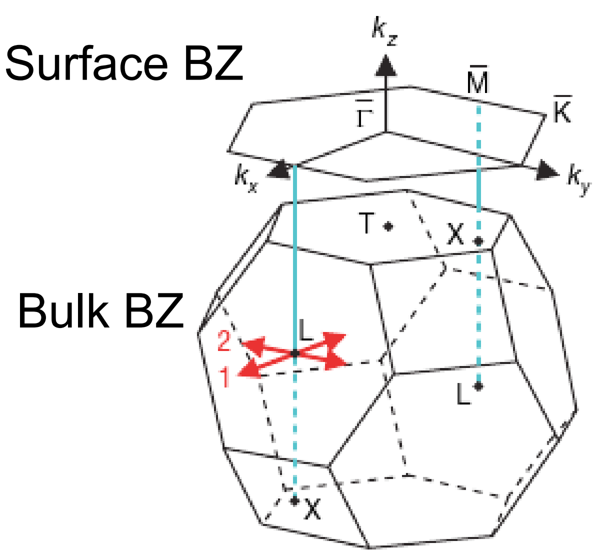
3D Strong T-I is found in experiments

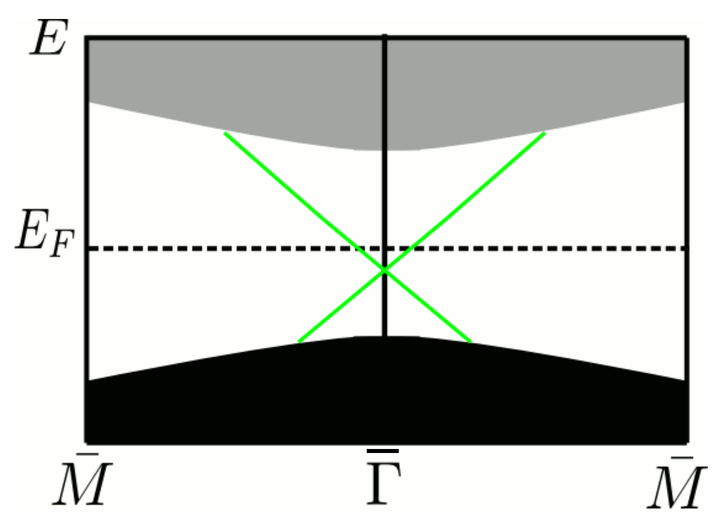
- $Bi_{1-x}Sb_x$

Theory: L. Fu & C. L. Kane (07)

- ARPES (Angle Resolved Photoemission Spectroscopy)

Directly measures surface electron dispersion.





Signature: Odd # of FS crossings from Γ to $\bar{M}$

3D Strong T-I is found in experiments

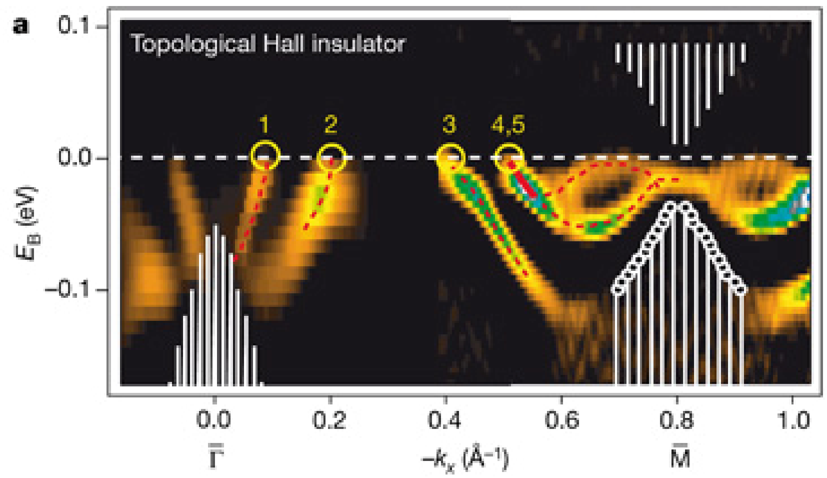
- $Bi_{1-x}Sb_x$

Theory: L. Fu & C. L. Kane (07)

Surface modes ARPES confirms strong T-I.

Experiment: D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava and M. Z. Hasan, Nature (08)

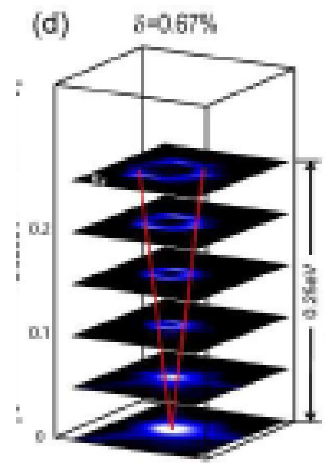
$$\nu_0 = 1; \mathbf{M}_\nu \propto (111)$$



5-crossings

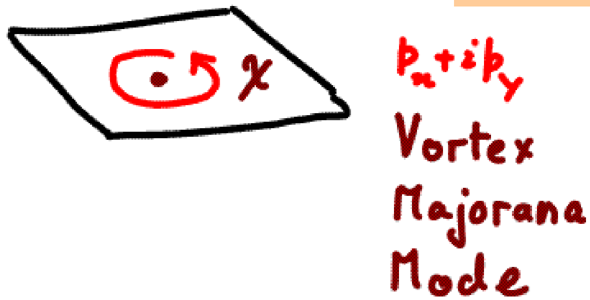
- New materials: Bi_2Se_3, Bi_2Te_3
  - Eg. Y. Chen et al. (2009).

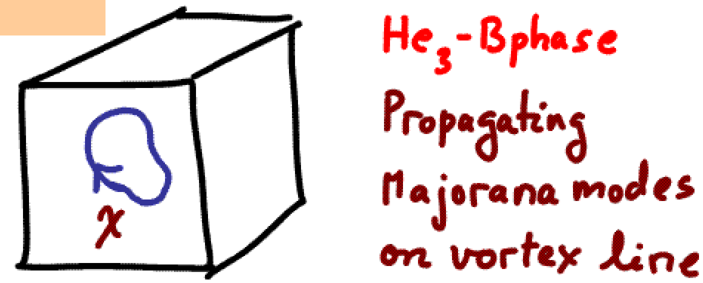
$$\nu_0 = 1; \mathbf{M}_\nu = 0$$



Broken Symmetry + Exotic Band Topology

- Superconducting order parameter: $|\Psi_0|e^{i\varphi}$
- Vortex defects: $\oint \nabla \varphi \cdot dr = 2\pi m$



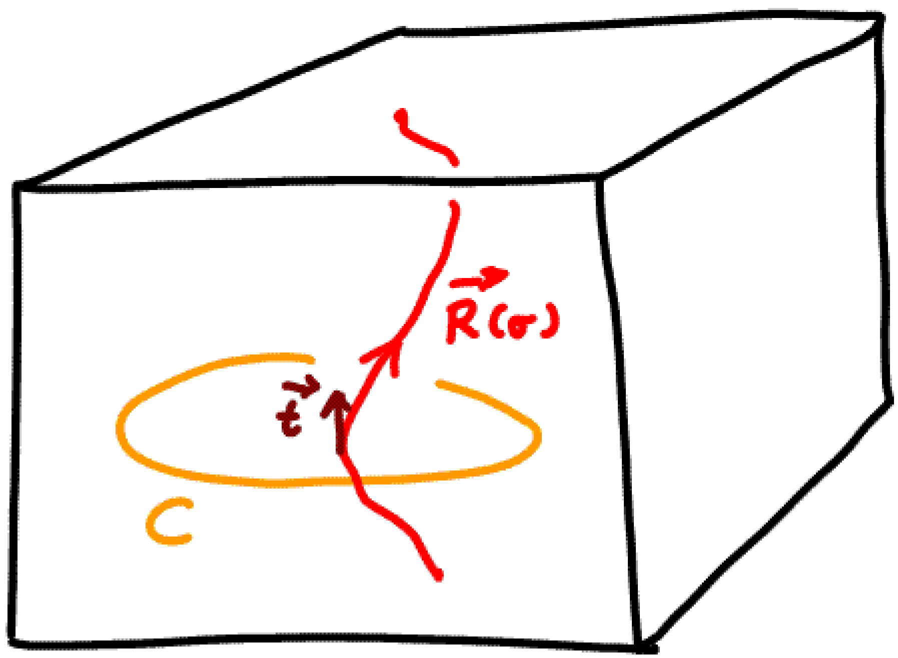


- Crystalline Solid – also broken symmetry phase.
  - Analog in topological insulators? YES
    - Dislocations host counter-propagating 1D modes. Like the edge of 2D QSH Insulator - Helical Metal.
    - Protected against disorder scattering – ideal quantum wire inside a bulk solid.

Line Defects in a Crystal

- Dislocations:

Defined by location **R**(σ) and 'strength' **B** .



$$\vec{r}_n = \vec{r}_n^{(0)} + \vec{u}(r_n)$$

↑ atom locations ↑ perfect crystal ↖ order parameter NOT single valued.

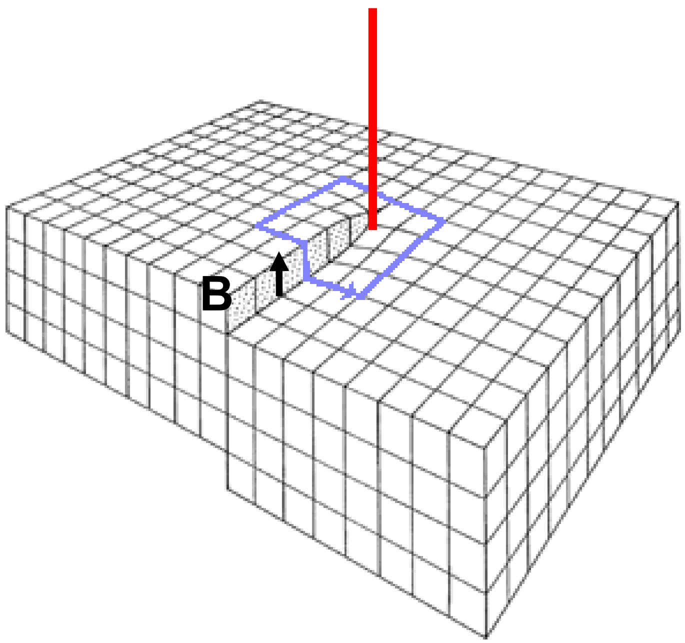
$$\oint_C d\vec{l} \cdot \vec{\nabla}\, \vec{u} = \vec{B} \ \{\text{a lattice vector}\}$$

B – Burgers Vector, must stay constant along the length and is quantized to lattice vectors. (Like vorticity)

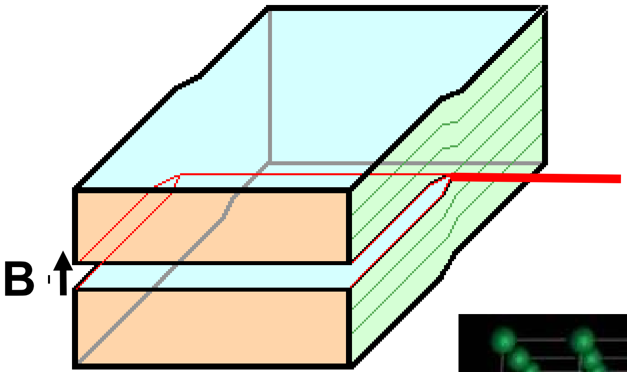
Visualizing Dislocations

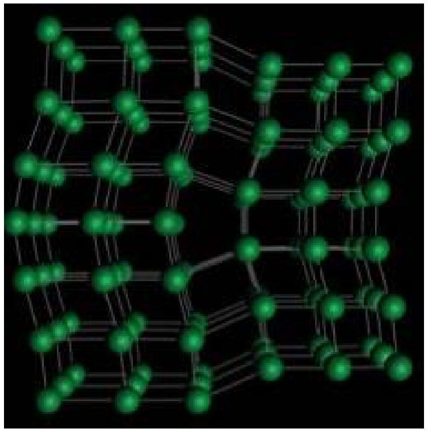
- Volterra Process:
  - Cut with an imaginary plane, that ends on the dislocation line **R**(σ)
  - Move all atoms on one side of the plane by the Burgers vector **B**
  - Add/remove atoms if required.

SCREW DISLOCATION: **t // B**



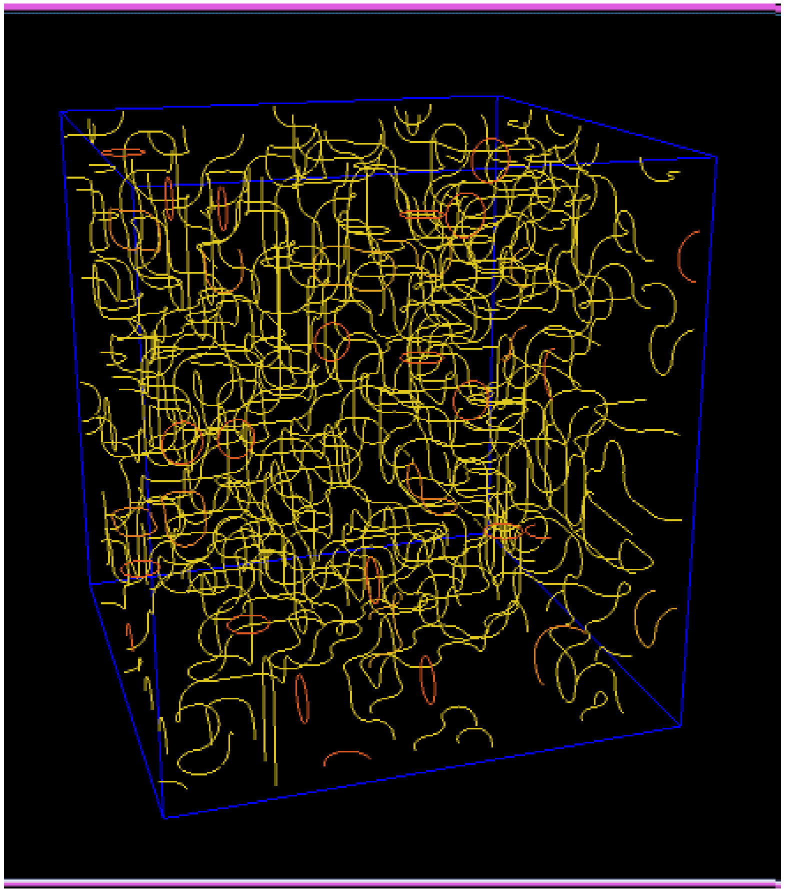
EDGE DISLOCATION: **t ⊥ B**

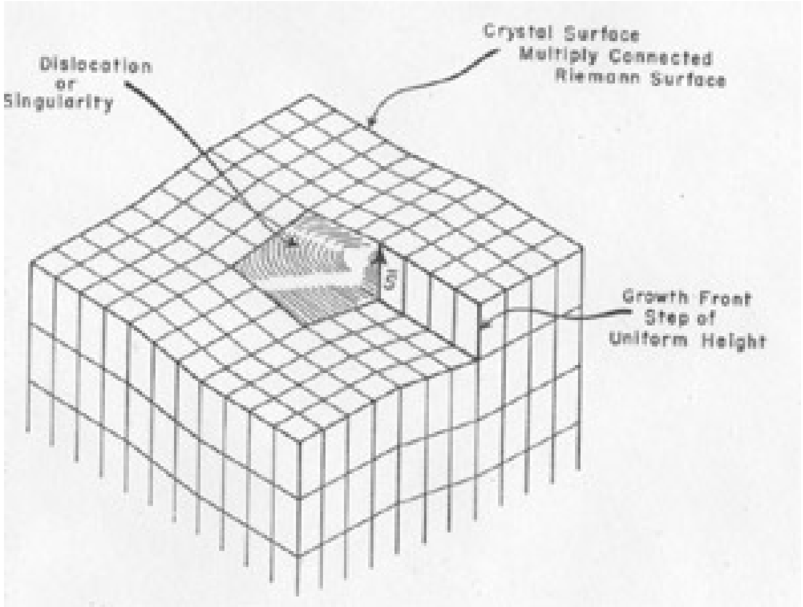




Dislocations in Solids

- Always present $\mathbf{n_d} \approx 10^{10} \mathbf{to}\, 10^{12} \mathbf{m^{-2}}$
- Control mechanical properties eg. Plastic Flow
- Crystal Growth – aided by screw dislocations.

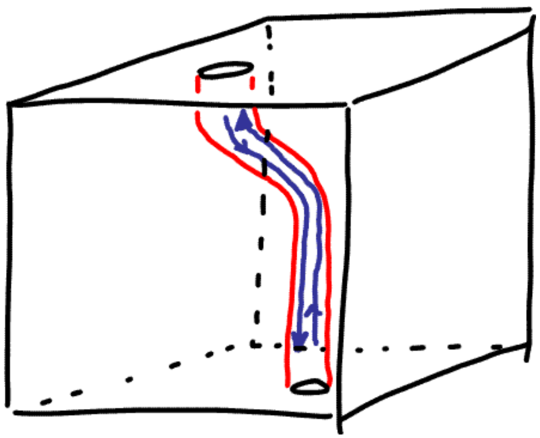


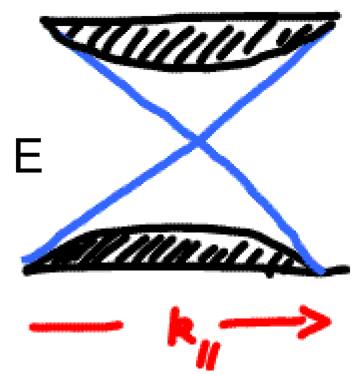


Dislocation in a Topological Insulator

- 1D Helical Metal occurs in a dislocation {**R**(σ), **B**} embedded in a topological insulator $\{\nu_0 = 0,1; \mathbf{M}_\nu\}$ iff:

$$\mathbf{B}\cdot\mathbf{M}_\nu = \pi \left(\mathrm{mod}\, 2\pi\right)$$

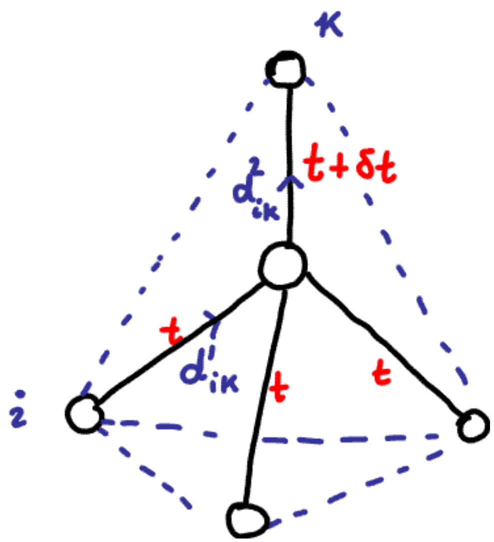




1D Modes are topologically protected:
•Cannot be gapped if Time Reversal Symmetry + bulk gap are present.
•Not localized by disorder
•Half of a regular quantum wire.

- Not all Top. Ins. have dislocation Helical modes. $\nu_0 = 1; \mathbf{M}_\nu = 0$
- Modes occur for both Weak and Strong Top.Ins.

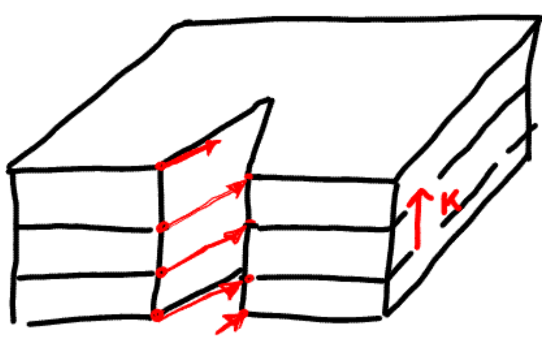
Illustration – Diamond Lattice Top. Ins.



$$H = t\sum_{\langle ij\rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + i\frac{\lambda_{SO}}{8a^2}\sum_{\langle\langle ik\rangle\rangle} c_{i\sigma}^{\dagger}(\vec{d}_{ik}^{1}\times\vec{d}_{ik}^{2})\cdot\vec{\sigma}_{\sigma\sigma'}c_{k\sigma'}$$

$$\nu_0 = 1; \mathbf{M}_\nu = \frac{\pi}{2}(1,1,1)$$

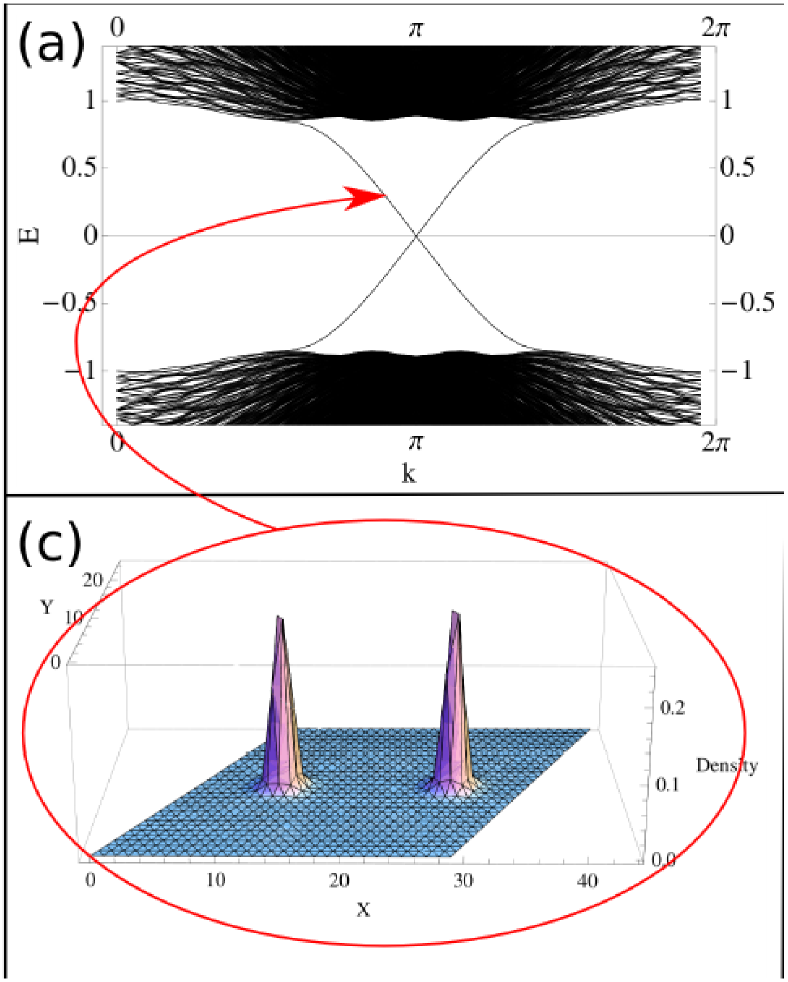
- Introduce a screw dislocation: **B**=(1,1,0).
  - Easily introduced in tight binding. Momentum dependent phase factor for cut bonds.



$$t \to t\, e^{\pm i\vec{K}\cdot\vec{B}}$$

Results: Screw Dislocation in Diamond Lattice Top. Ins.

- Insert a pair of screw dislocations (36x36x18 periodic BC). Momentum along the dislocations is a good quantum number.
- Two propagating modes per dislocation. `Helical metal'.

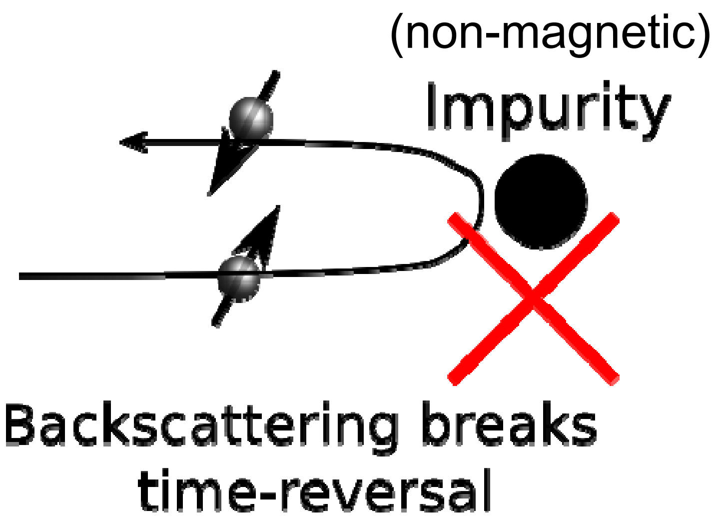


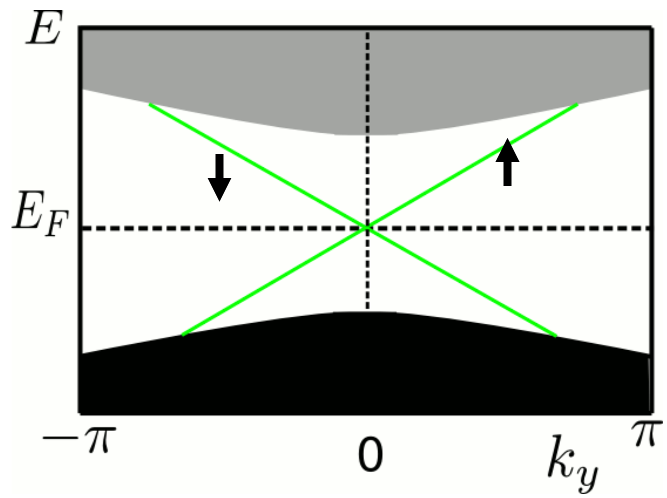
Absence of localization

- Stable to disorder:

(TR symmetry ➡ no backscattering)

An atomically thin one dimensional wire that does *not* localize.

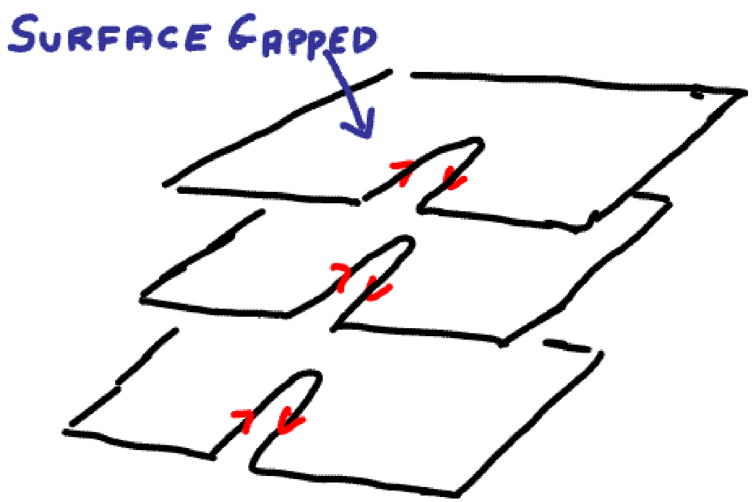




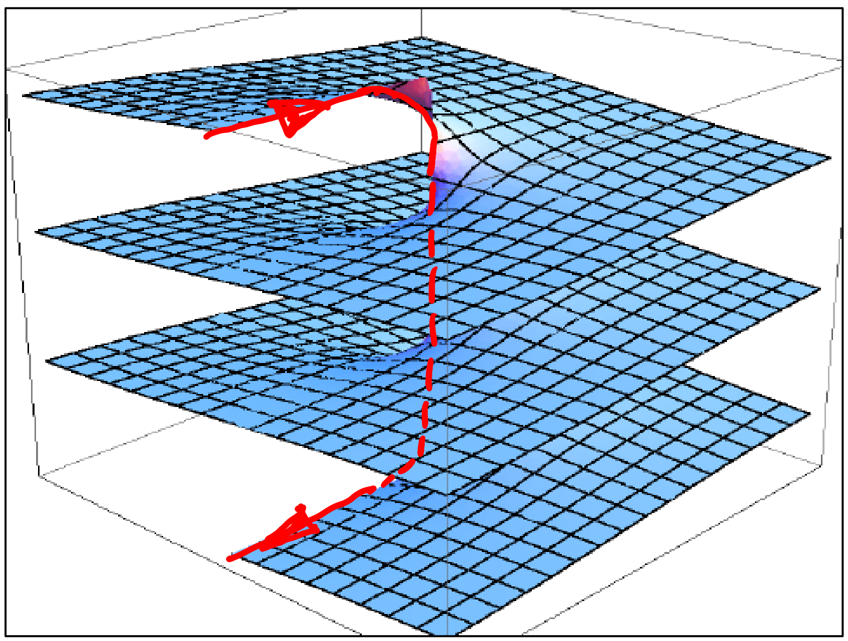
Similar to 2D quantum spin Hall edge states
With *strong* interactions, can spontaneously break time reversal symmetry, localization

Proof for Weak Top. Ins.

- Weak Top.Ins. Adiabatically connected to a stack of decoupled 2D Top.Ins.,
  - stacking along $\mathbf{M}_\nu$
  - Different proof for Strong TI

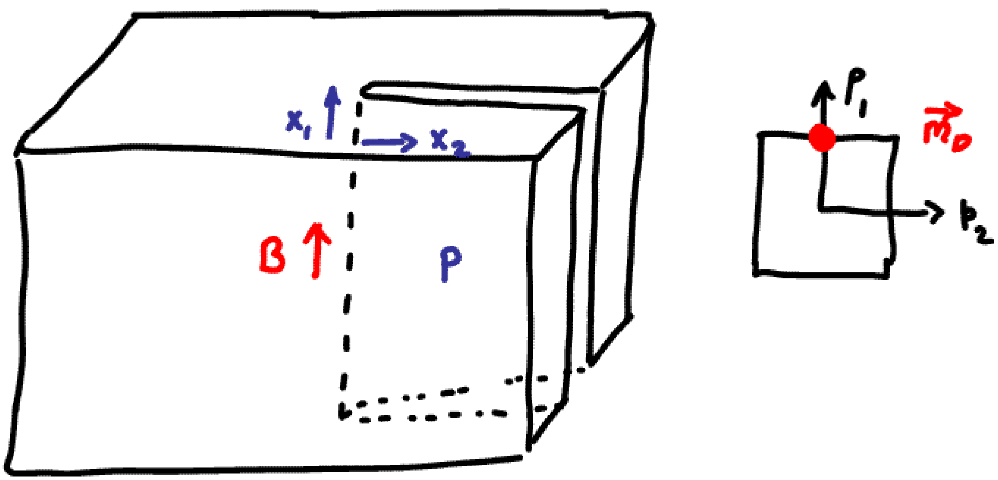


Cut Surface – only one of the helical mode pairs is shown.



Glued Surface – Dislocation must carry helical modes

Proof For General Top. Ins. 1



- Screw dislocation – **if** surface Dirac node is at momentum $\mathbf{m}_{\mathrm{Dirac}} \cdot \mathbf{B} = \pi$ then (-1) phase acquired on crossing the dislocation.
- In the weak surface connection limit => Dirac equation that changes mass term sign.

$$H = \left(p_1\sigma_1 + p_2\sigma_2\right)\mu_z + m(x_2)\mu_x$$

$$m(x_2 > 0) = -m$$
$$m(x_2 < 0) = +m$$

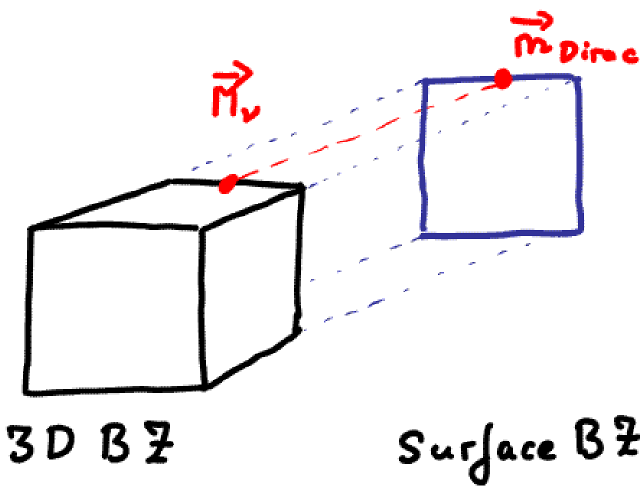
Proof For General Top. Ins. 2

$$H = (p_1\sigma_1 + p_2\sigma_2)\mu_z + m(x_2)\mu_x$$

$$m(x_2 > 0) = -m$$
$$m(x_2 < 0) = +m$$

- Pair of zero modes at p_1=0. $\psi(x_2) = \psi_0 e^{-\int_0^{x_2} |m(x')| dx'}$
- Propagating 1D helical modes for general p_1.

- Location of Surface Dirac Node – controlled by $\mathbf{M}_\nu$



$$\mathbf{m}_{\mathbf{Dirac}} \cdot \mathbf{B} = \pi$$
$$\Downarrow$$
$$\mathbf{M}_\nu \cdot \mathbf{B} = \pi \pmod{2\pi}$$

Experimental Signatures

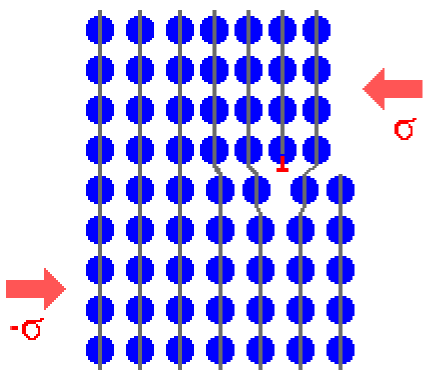
- Resistivity: dislocation contribution could dominate over surface conduction.

$$\rho = \frac{h}{2e^2}\frac{1}{l\,n_d} \approx 10^{-2}\,\Omega\mathbf{m} \qquad n_d \approx 10^{12}\,m^{-2} \qquad l \approx 1\mu m$$

(in current samples – impurity band conduction dominates)

Experimental Signatures

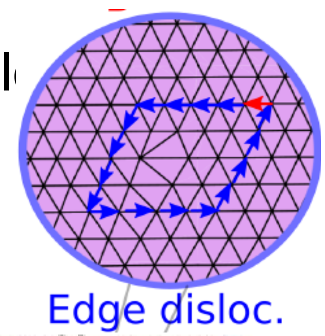
- Dislocations can be created during plastic deformation. For the right kind of stress (connected to lattice indices $\mathbf{M}_\nu$) increased conductivity.



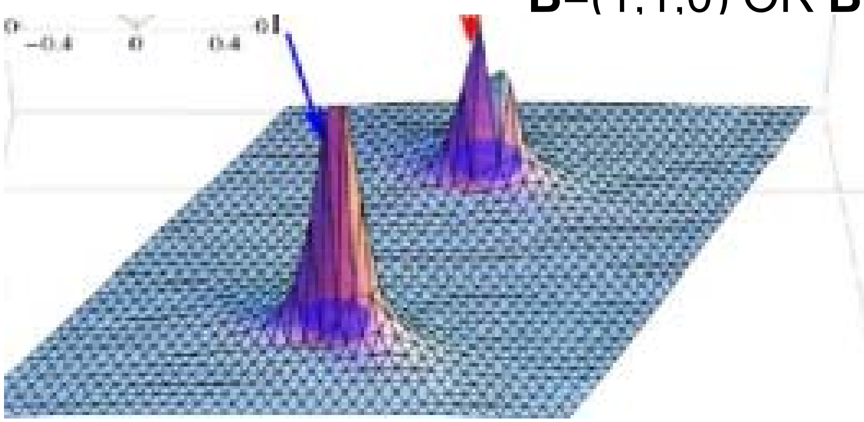
Experimental Signatures - STM

- Can determine atomic defect structure and Local Density of States (LDOS).
  - 1D modes – finite DOS. (ideally operate at Dirac point with vanishing density of states)

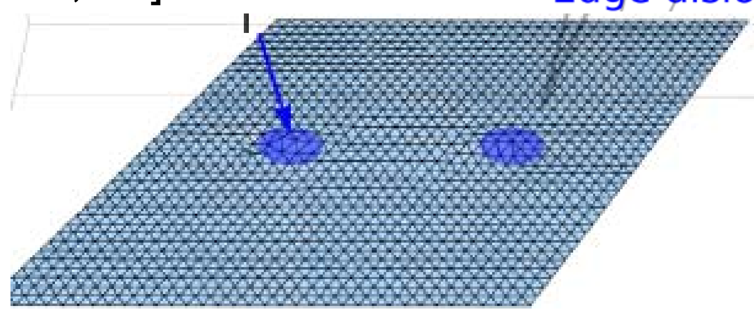
- Demonstration - Diamond lattice strong Top.Ins.. Edge disl



Edge dislocation on (-1,-1,1) Surface.
B=(1,1,0) OR **B**=(-1,0,1).
S in [-0.1,0.1].



$\mathbf{B}\cdot\mathbf{M}_\nu = \pi$



$\mathbf{B}\cdot\mathbf{M}_\nu = 0$

Effect of Lattice Disorder

- Very Strong Disorder – dislocations proliferate; no meaning to $\mathbf{M}_\nu$

- Moderate disorder – dilute dislocation density. Can still characterize using gapless modes in dislocations and define $\mathbf{M}_\nu$. Weak insulators can be defined even *with* disorder.

  but Surface states localized.

(weak insulators can be defined *even* when surface states localized)

Conclusions

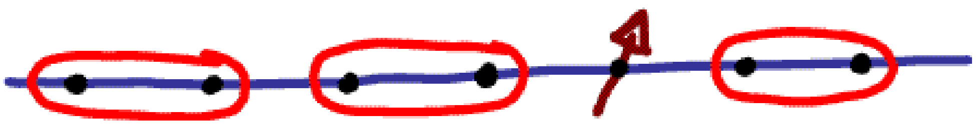
- 3D topological Band Insulator has protected helical mode in those dislocations that satisfy

$$\mathbf{B}\cdot\mathbf{M}_{\nu} = \pi \left(\mathrm{mod}\, 2\pi\right)$$

Should occur in $Bi_{1-x}Sb_x$ $\mathbf{M}_{\nu} \propto (111)$ but not in Bi_2Se_3, Bi_2Te_3 $\mathbf{M}_{\nu} = 0$

- Indicates weak topological insulator stable to disorder if dislocations do not proliferate.
- Another example of a `dressed' topological defect – intrinsically quantum phenomena.

Eg: Dimerized spin ½ chain.
Domain walls carry spin



When defects are quantum mechanical – leads to new phases and phase transitions