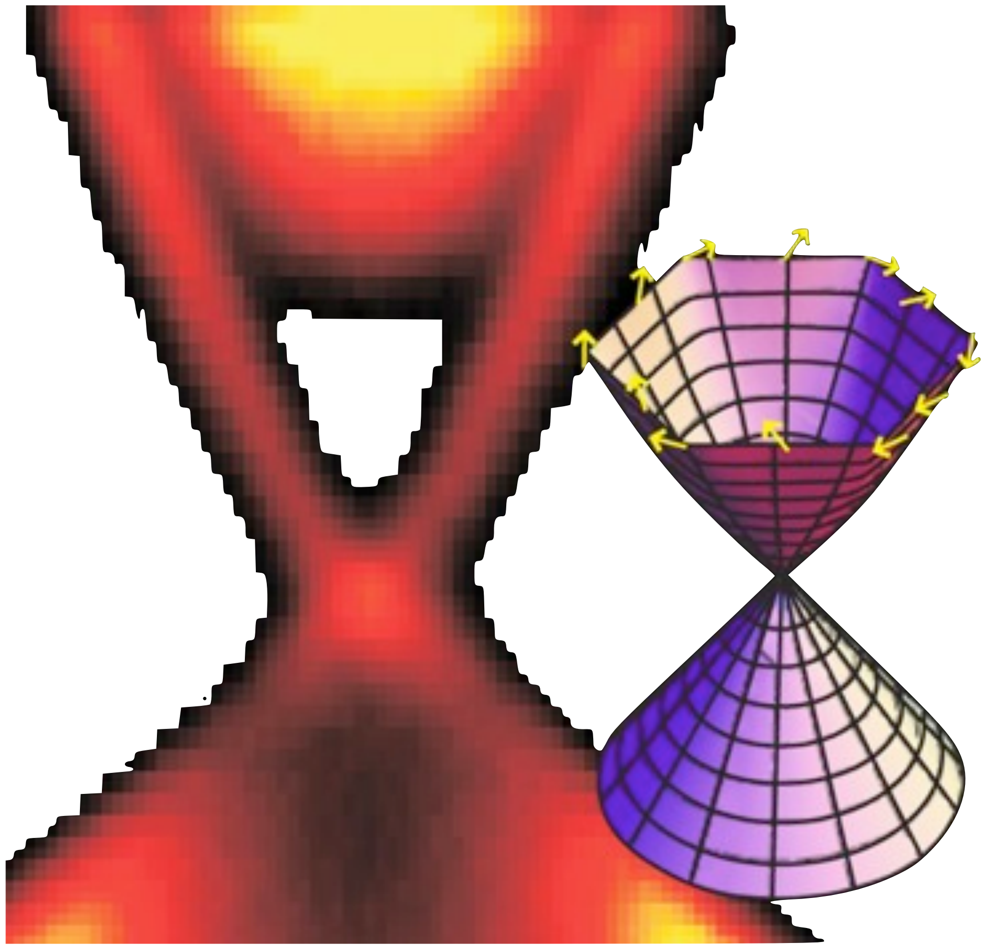
Introduction to Topological Insulators



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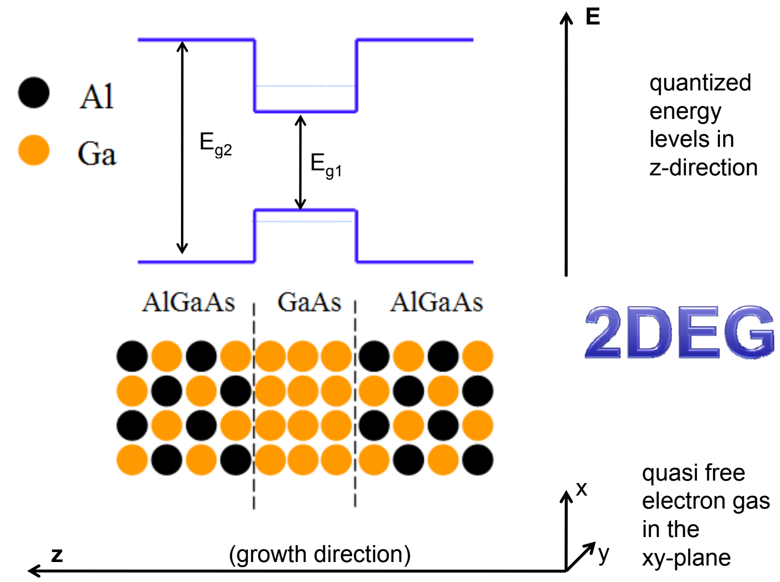
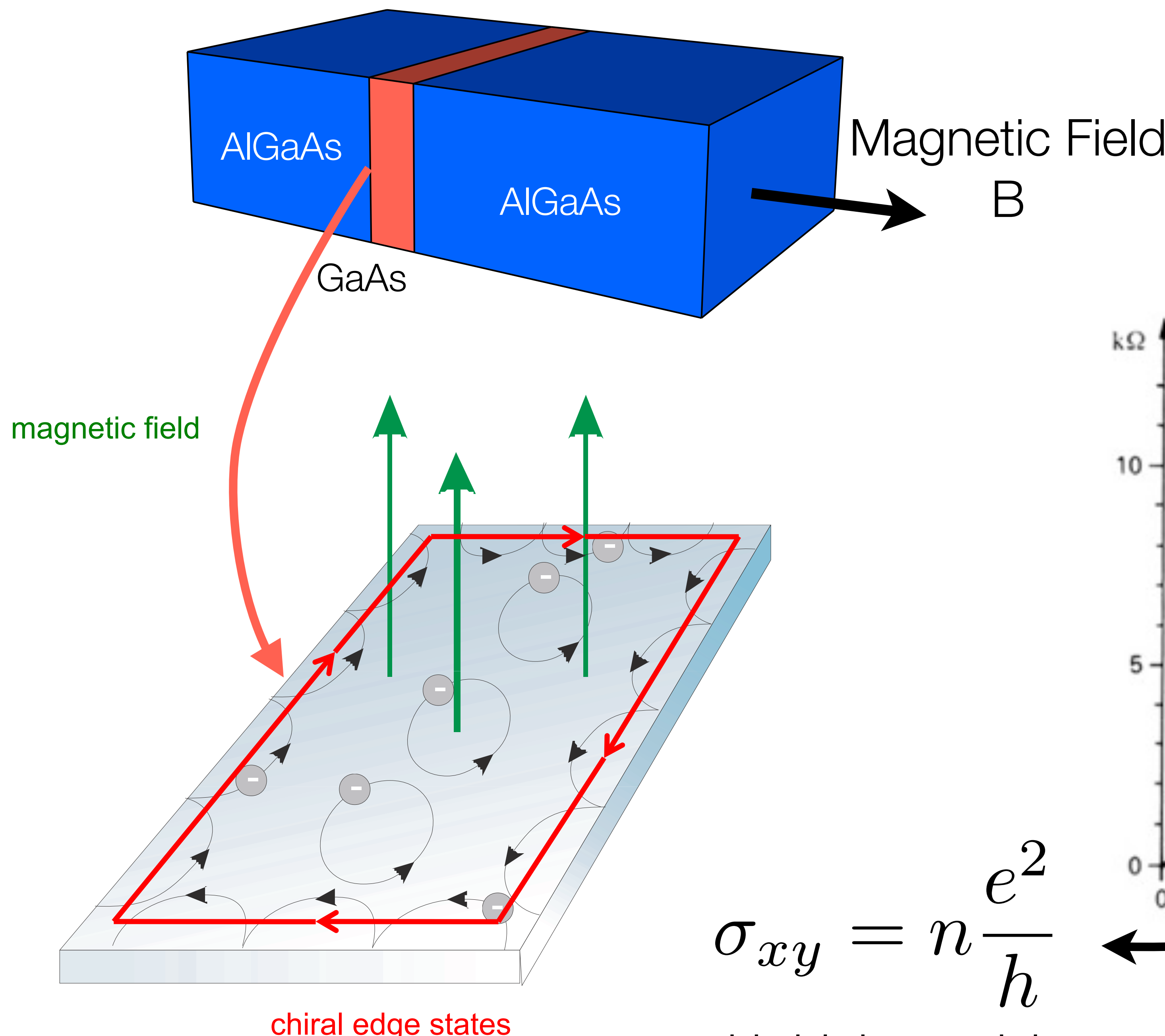
Berkeley : J. Moore, A. Vishwanath

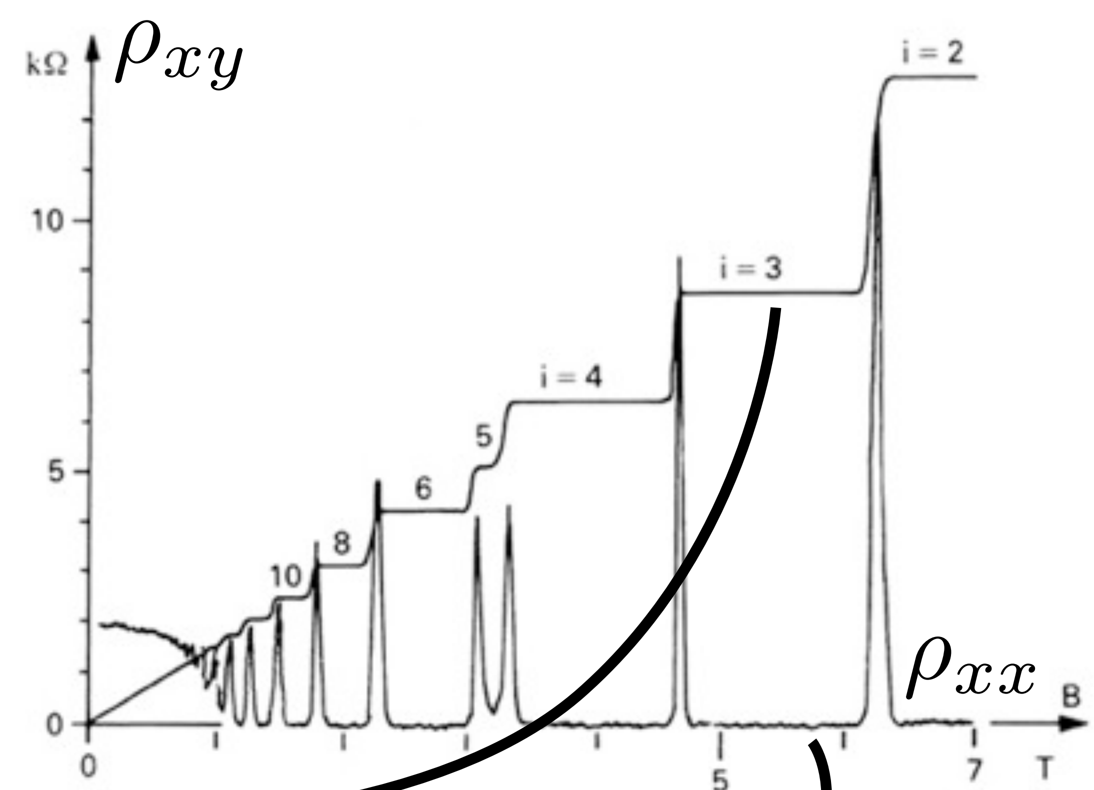
CERN, Jan. 2011

(Integer) Quantum Hall Effect : Anomalous Insulator

- 2DEG (Heterojunction GaAs/AlGaAS)





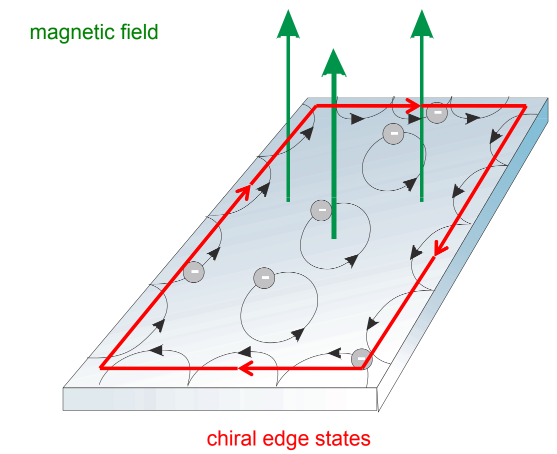


$$\sigma_{xy} = n\frac{e^2}{h}$$

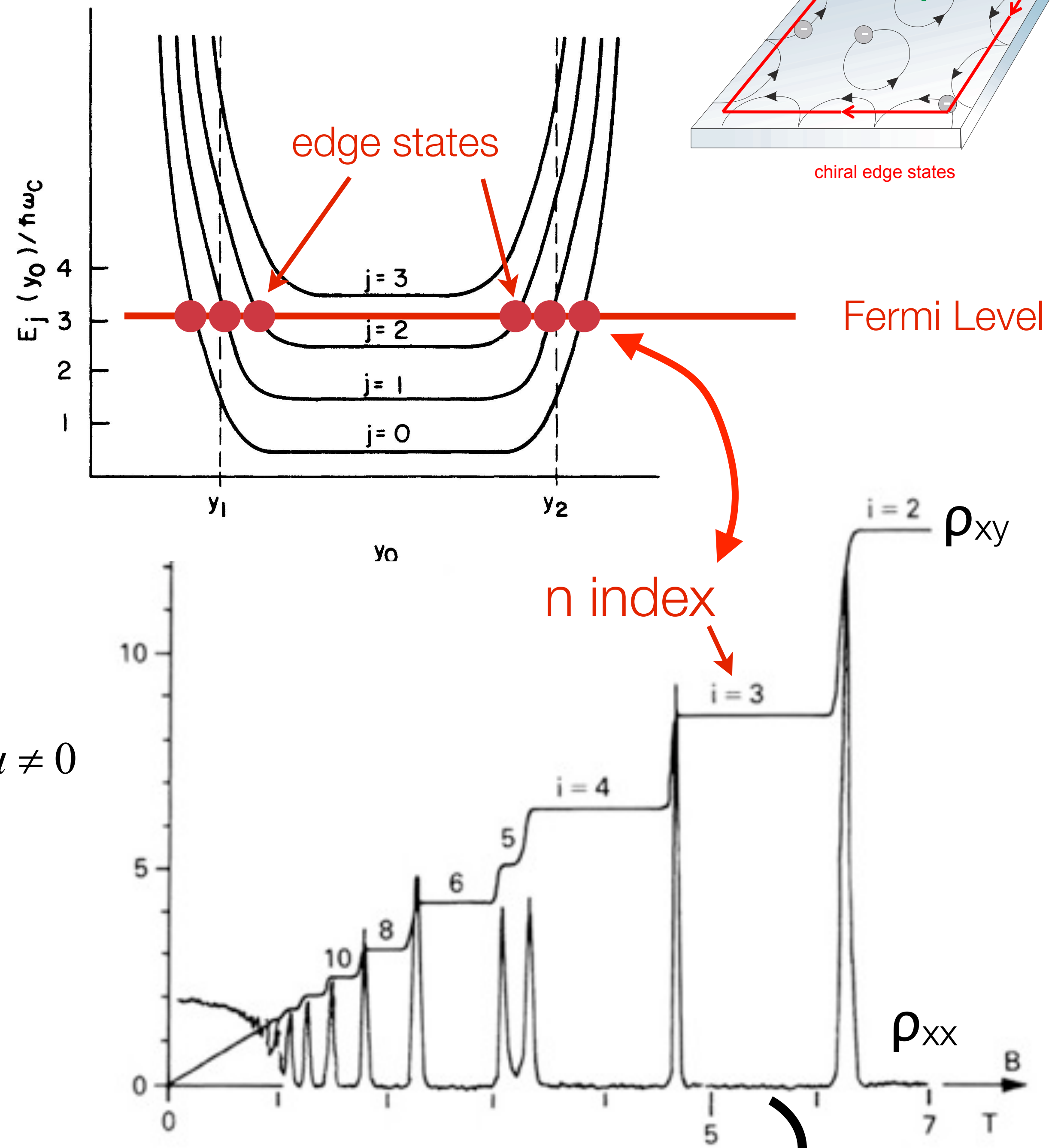
with high precision

No longitudinal resistivity : Insulator

Quantum Hall Effect : the edge states

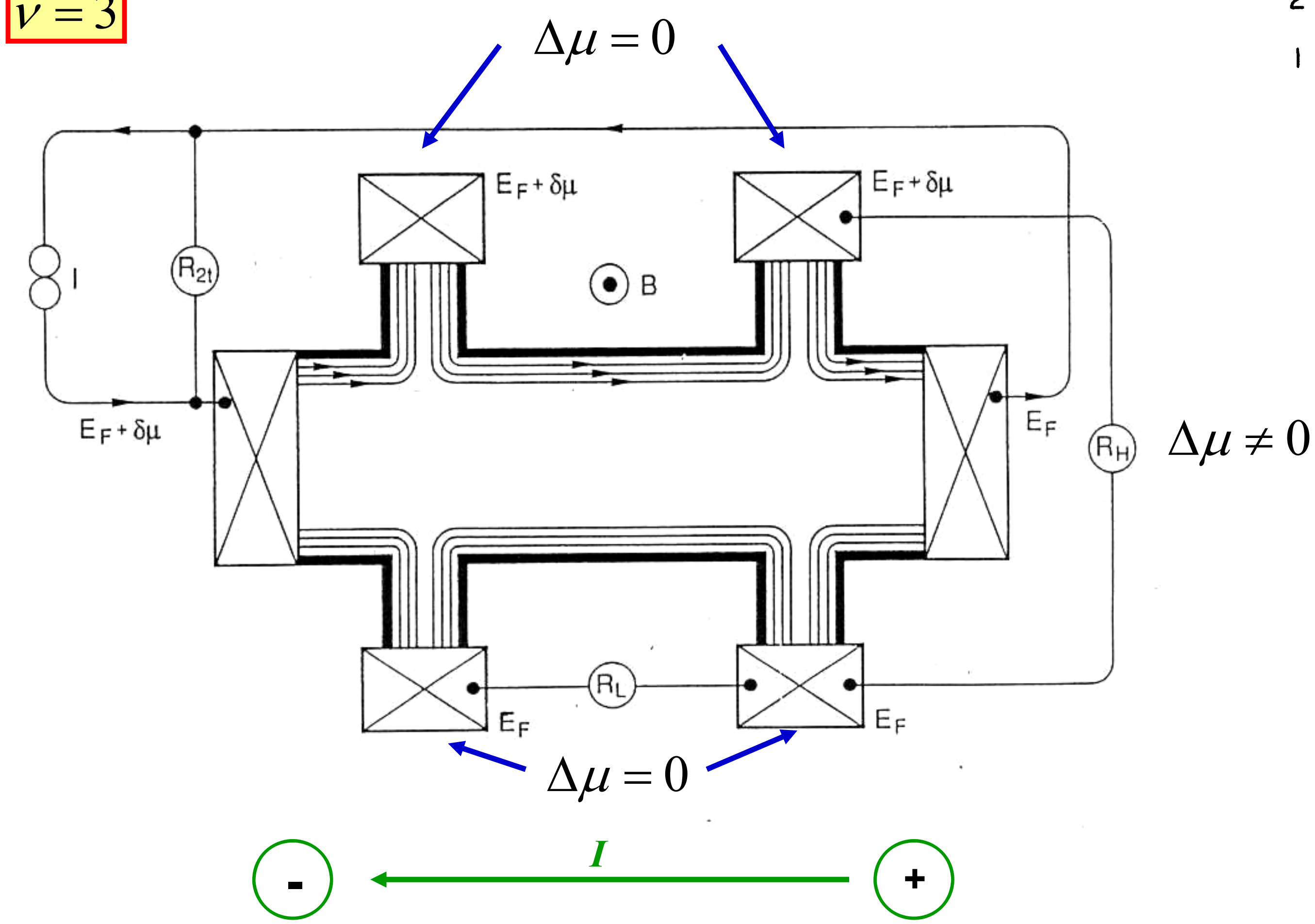


Transport Properties of Quantum Hall Effect: described by Edge States
➡ Complete characterization of IQHE



$\nu = 3$

Edge Channel Picture



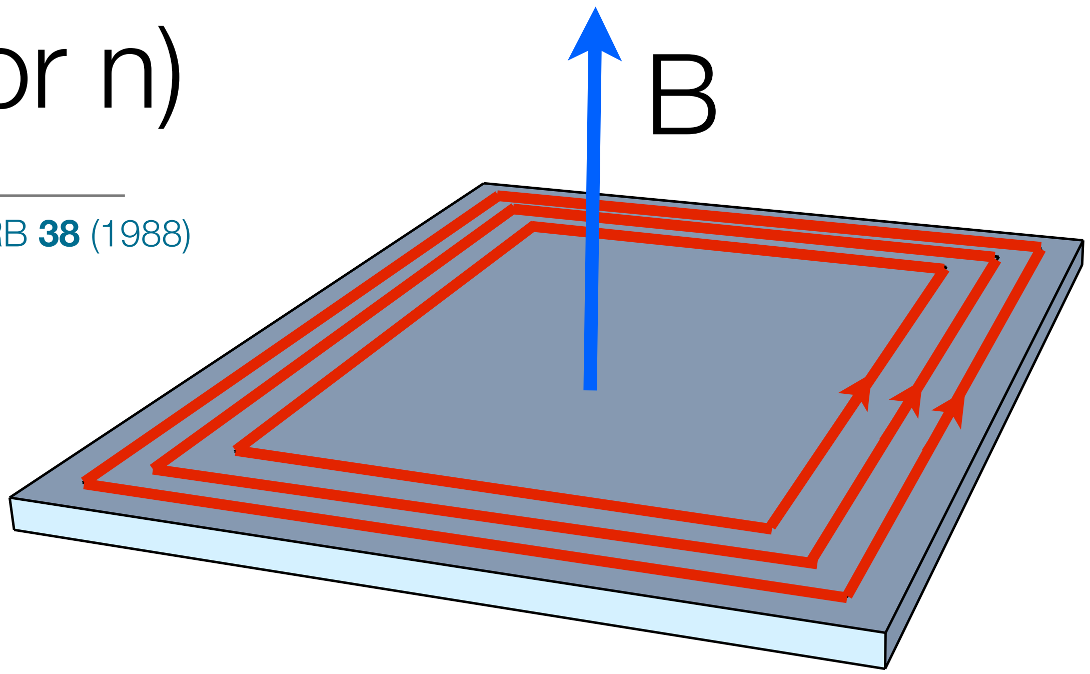
Chirality + n →conductance matrix → multi-terminal conductances

No longitudinal resistivity : Insulator

M. Büttiker, PRB **38** (1988)

Robustness of edges states (or n)

M. Büttiker, PRB **38** (1988)



Quantum Hall Effects :

- break Time reversal symmetry (by **B**)

➡ edges states are chiral

- integer n ⇒ counts number of edge modes
- edges modes come by pair (spin symmetry)

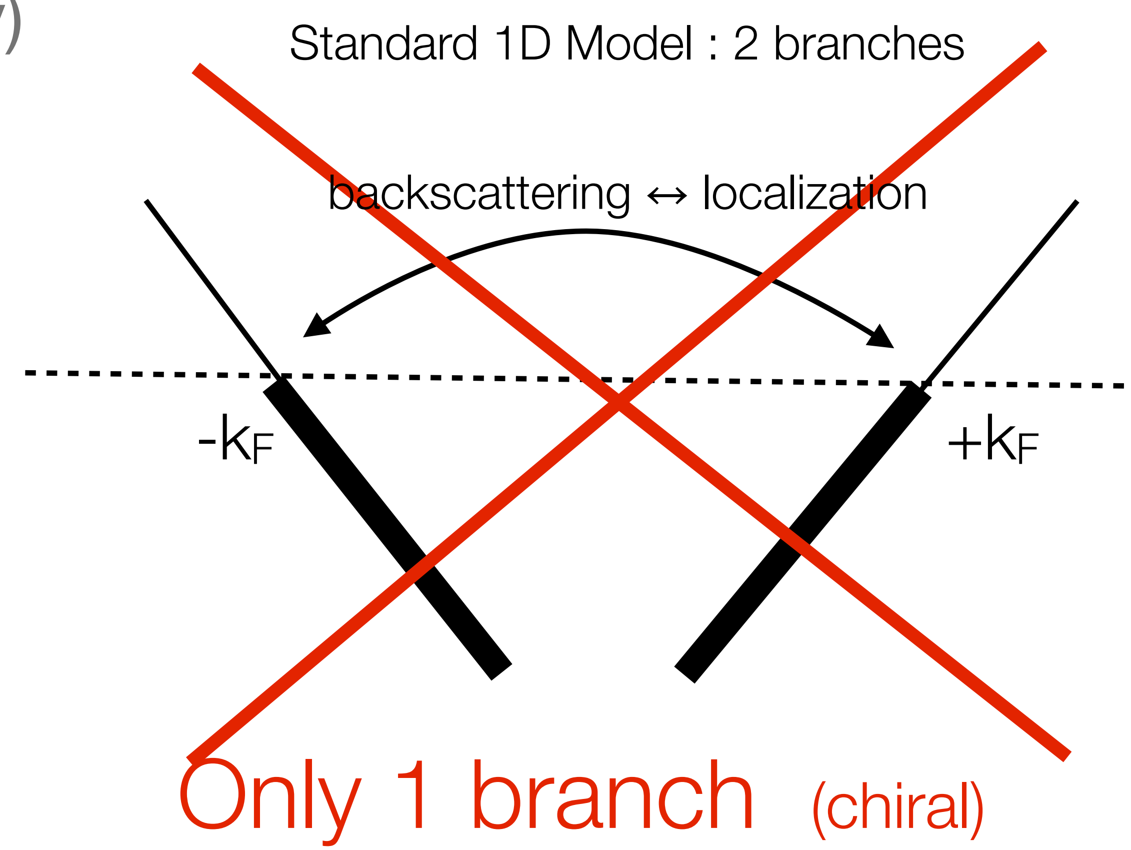
Robustness of edge states :

no backscattering because chiral modes

⇒ all n modes are ballistic

Robustness of n : chirality of the modes (T-breaking)

no possible generalization ?



Quantum Hall Effect : a Topological Insulator

Thouless *et al.*. PRL **49** (1982)

$$\sigma_{xy} = n\frac{e^2}{h}$$

Alternative description : n is a topological invariant

Describes properties of an insulator (gap necessary)

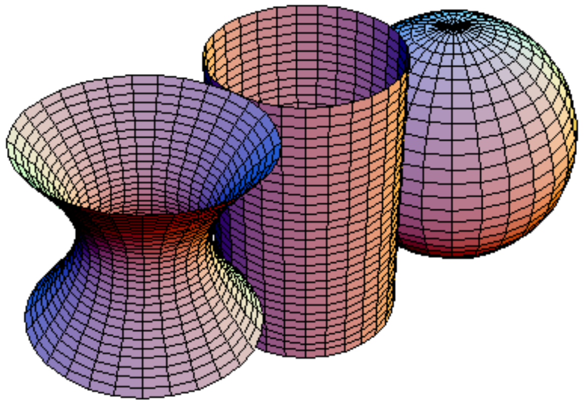
Property of the filled band / ensemble of 1 particle waves functions $(u_m(\mathbf{k}))$

Insensitive to small changes of the filled band / Hamiltonian :

- disorder
- geometry
- weak interactions
- etc

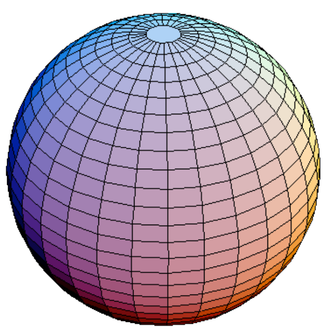
➡ Notion of Topological Insulator

Topological invariant ?

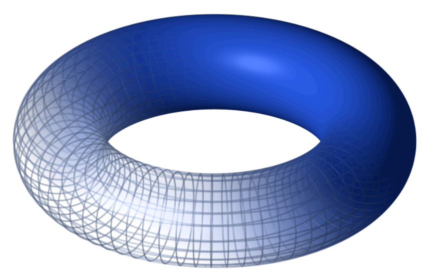


Gaussian curvature : $\kappa = 1/(R_1 R_2)$

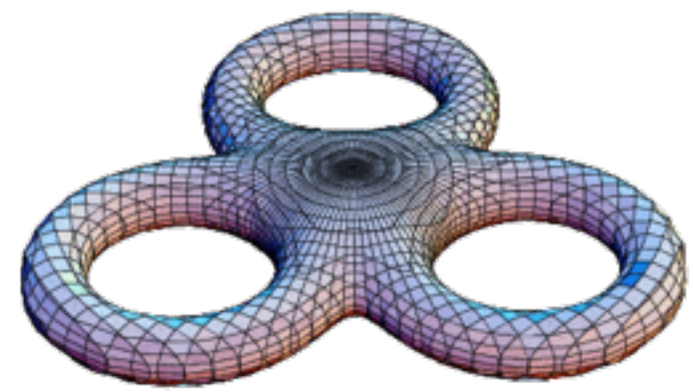
For closed surface : Gauss-Bonnet theorem



$g = 0$



$g = 1$



$g = 3$

$$\int dS \ \kappa = 2\pi(2 - 2g)$$

Integral of curvature : depends only on «global properties» (topology), insentitive to small changes / deformation of surface

for more complex surfaces (vector bundles) : chern numbers

Quantum Hall Effect : TKNN invariant

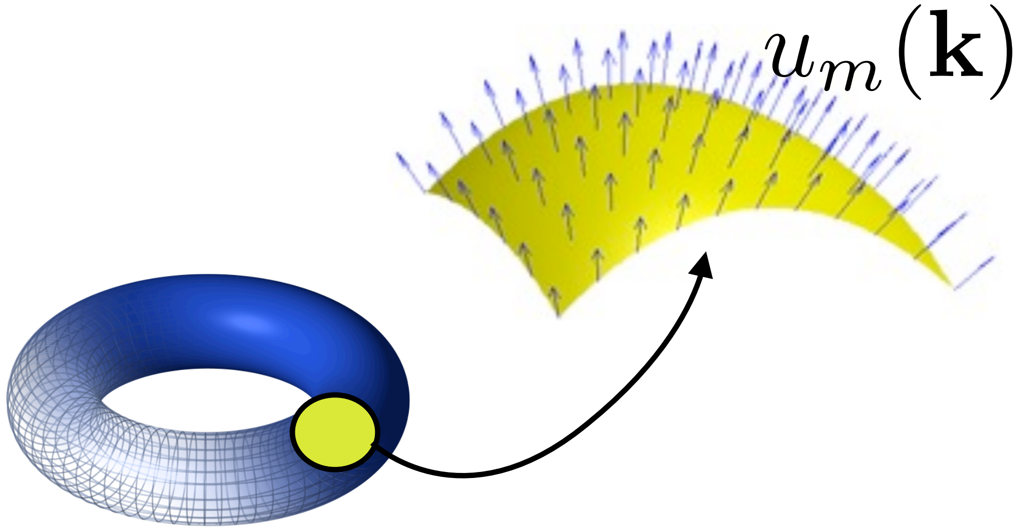
Thouless *et al.*. PRL **49** (1982)

- Bulk Gap ⇒ focus on Ground State $(u_m(\mathbf{k}))$

- Topological Order : the TKNN invariant

$$\sigma_{xy} = n\frac{e^2}{h} \qquad n = \frac{1}{2\pi}\int_{BZ} d^2\mathbf{k}\ \underbrace{\nabla \times \mathcal{A}}$$

(Berry's) curvature



Brillouin Zone

$$\mathcal{A} = i\sum_m \langle u_m|\nabla_{\mathbf{k}}|u_m\rangle$$

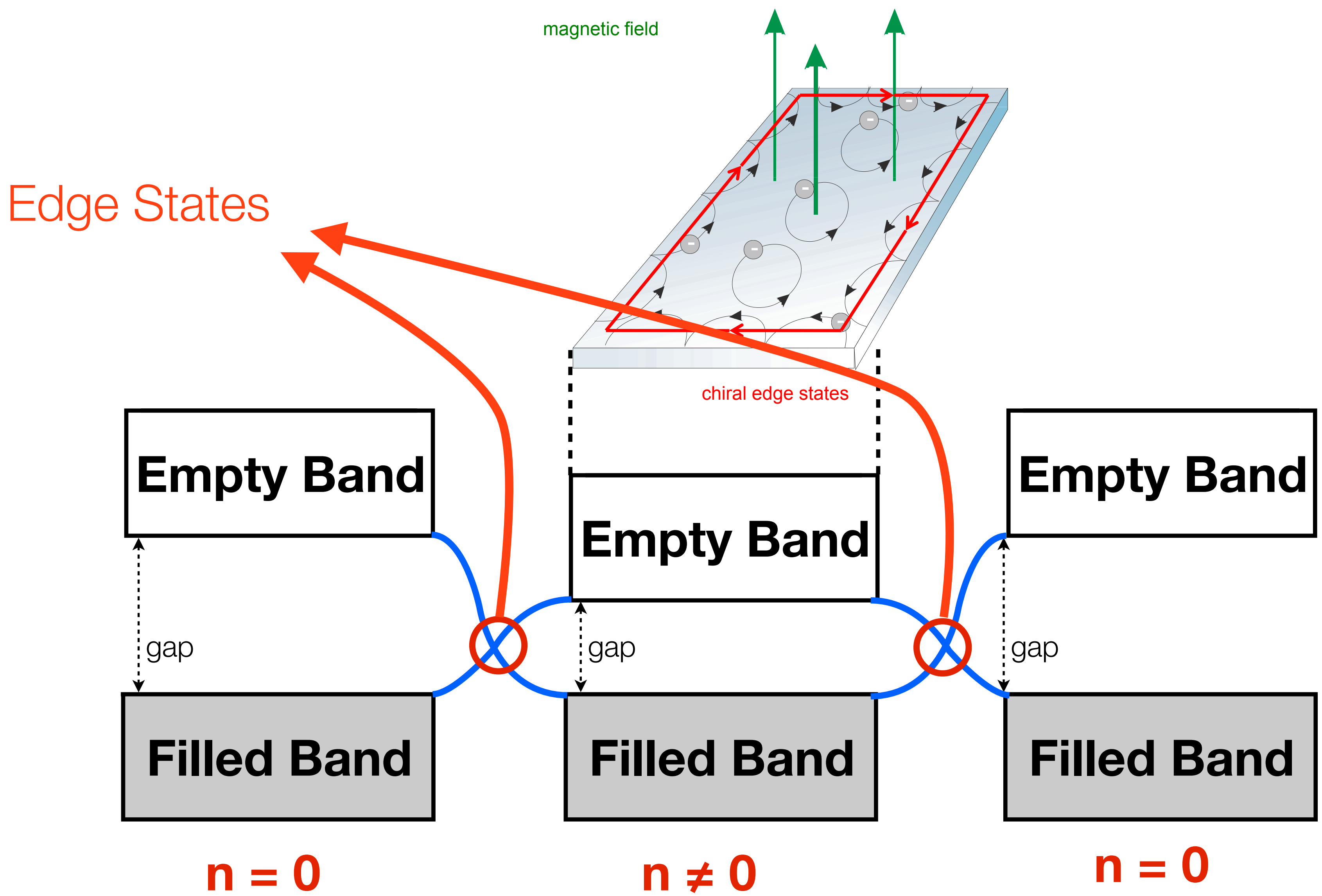
$u_m(\mathbf{k})$: 1 particule state of occupied band

n : integral of curvature = topological (Chern) number

- σ_{xy} is given by a topological number

➡ insensitive to perturbations of the $u_m(\mathbf{k})$ (or Hamiltonian)

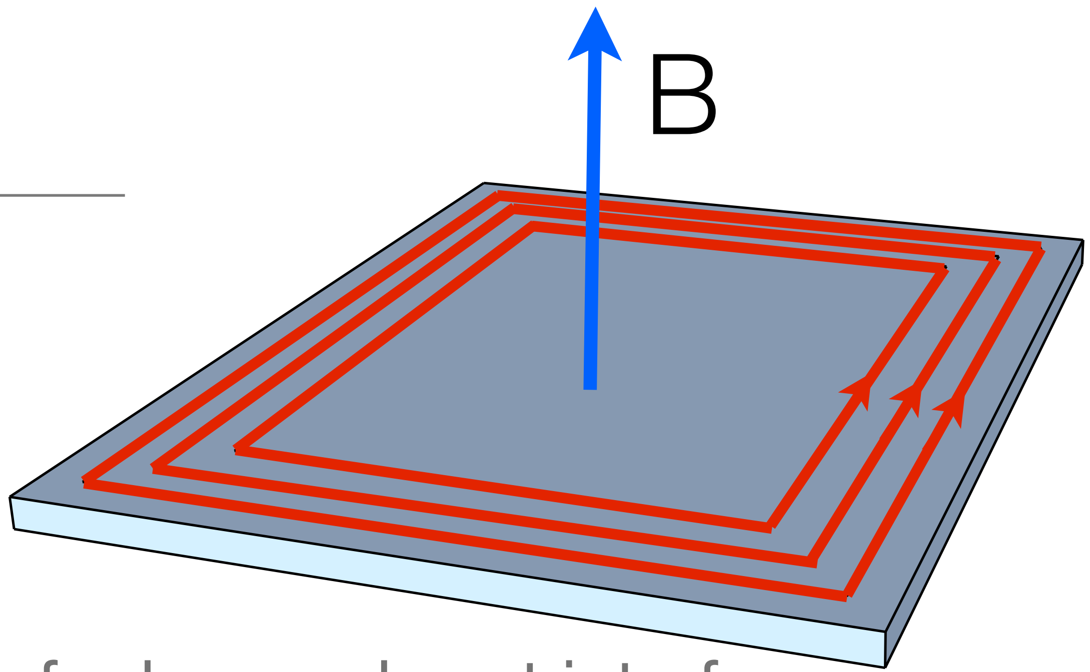
Topological order ⇔ (robust) edge states



Topological invariant : **n**

Robustness of top. invariant n
↔ robustness of edge states (edges remain ballistic)

Other topological insulators ?



Quantum Hall Effects :

- break Time reverseal symetry (by B)

➡ edges states are chiral

- top invariant : integer n ⇒ counts number of edge modes at interface
- edges modes come by pair (spin symmetry)

T reversal breaking necessary for topological insulators ?

No ⇒ new class of topological insulators discovered

(no T breaking)

1. New 2D phase : Quantum Spin Hall Effect
   - proposed theoretically in 2005 — Kane and Mele, PRLs **95** (2005); Bernevig, Hugues and Zhang, Science **314** (2006)
   - found experimentally in 2007 — König *et al.*, Science **318** (2007)
2. New 3D phase : 3D Topological Insulators
   - proposed theoretically in 2007 — Fu, Kane et Mele, PRL **98** (2007); Moore and Balents, PRB **75** (2007); Roy, PRB **79** (2009); Fu and Kane, PRB **76** (2007)
   - Experimental tests in 2008 — Hsieh *et al.*, **95** (2008)

New topological insulators : Spin Orbit Induced

Crucial ingredient : spin orbit interaction

$$H_{SO}^{eff} = \lambda(\mathbf{p} \times \nabla V).\mathbf{S}$$

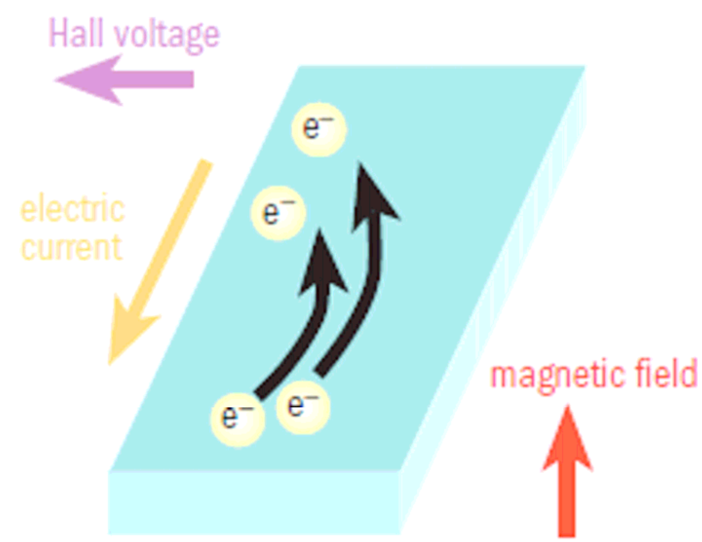
- momentum dependent force : for fixed spin, analogous to magnetic field **B**
- opposite force for opposite spins
- energy ±μB depending on spin of electrons
- spin-orbit strongly enhanced for atoms of large Z (look at the bottom of table)

- T reversal symmetry : reverses both **p** and **S** !

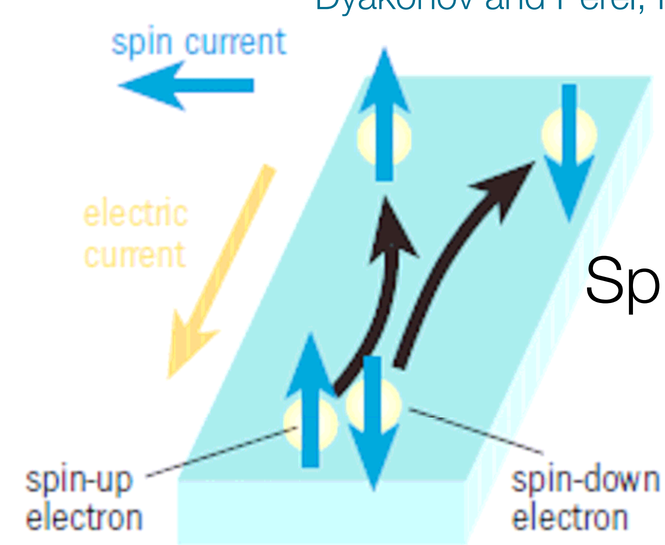
  ➡does not break T-reversal symmetry

- first consequence : spin hall effect

Dyakonov and Perel, Phys. Lett. **35A** (1971)



Hall effect

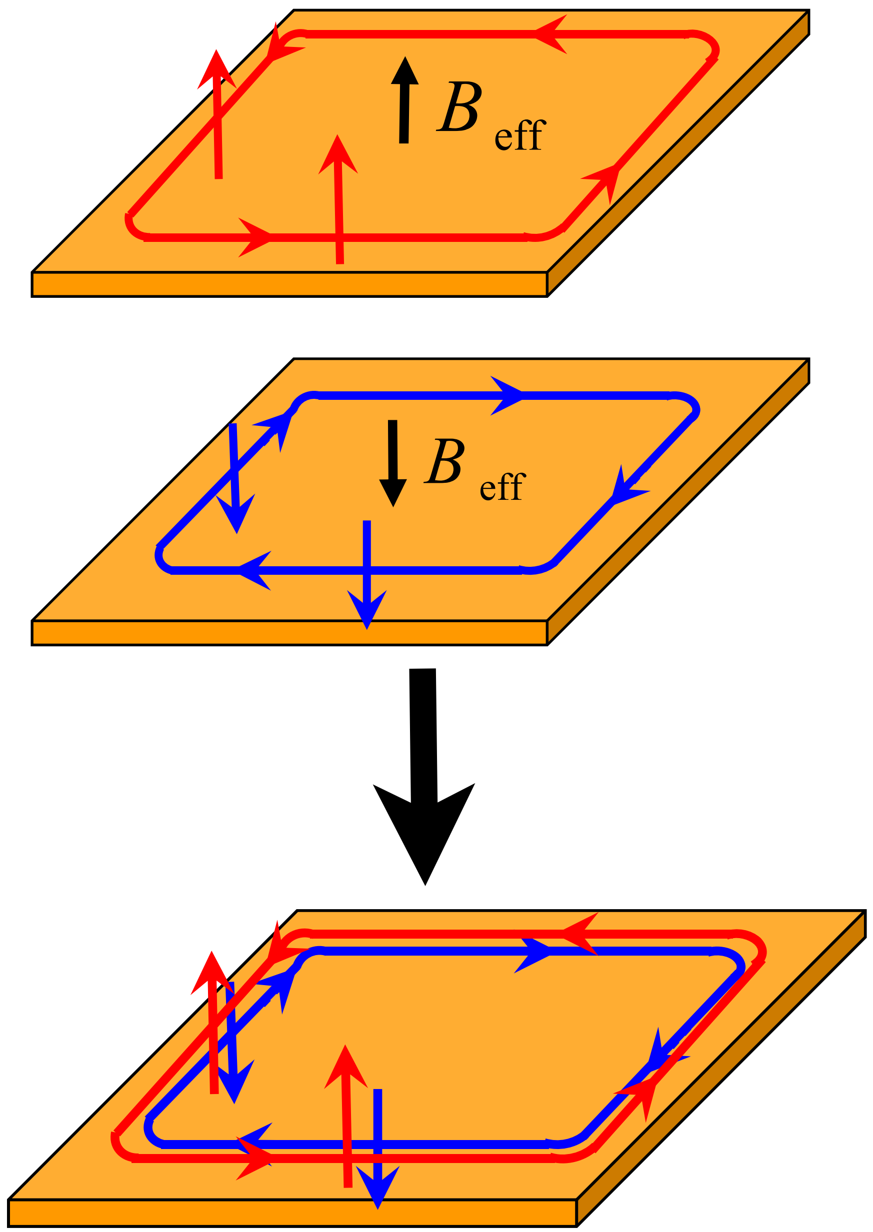


Spin Hall effect

Quantum Spin Hall Effect = 2 copies of IQHE

C.L.Kane and E.J.Mele, PRL 95, 226801 (2005)
B.A Bernevig, T.L. Hughes, S.C. Zhang, Science 314, 1757 (2006)

- For strong enough SO interaction in 2D :
- 2 copies of IQHE with opposite magnetic field B_{eff}. One for each spin.
- Insulating bulk (for each spin)
- Does not break Time Reversal Symmetry (exchange spin and momentum)



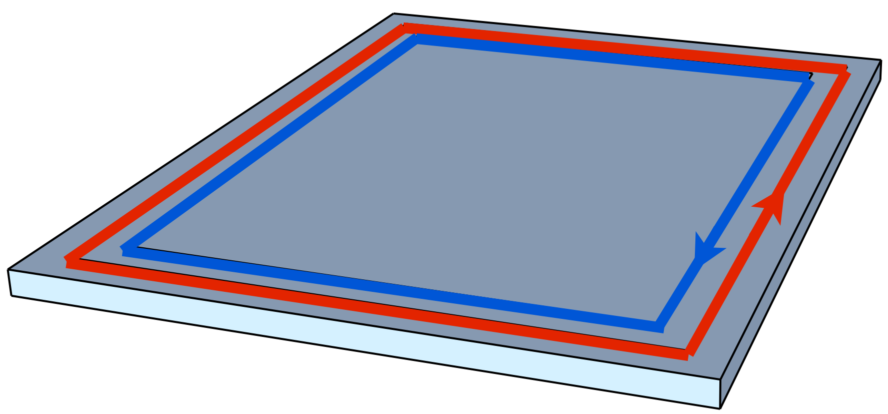
.. But need to open the gap for each spin in the first place !

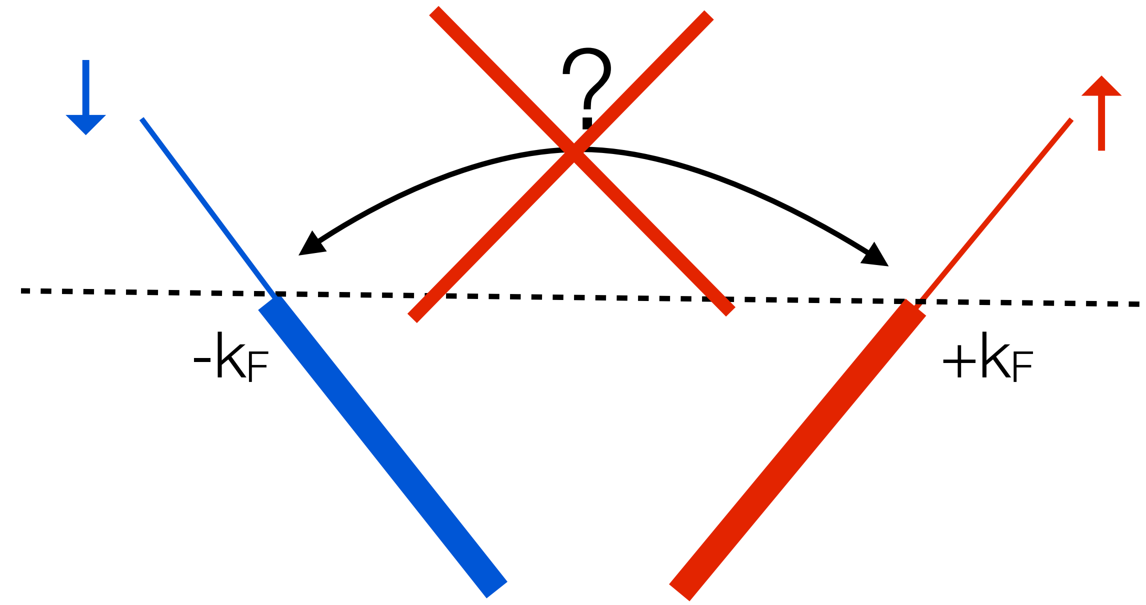
Quantum Spin Hall Effect : Topological Order

C.L.Kane and E.J.Mele, PRL 95, 226801 (2005)

- «Protected Edge States» : robust properties, remain ballistic

with 2 modes :

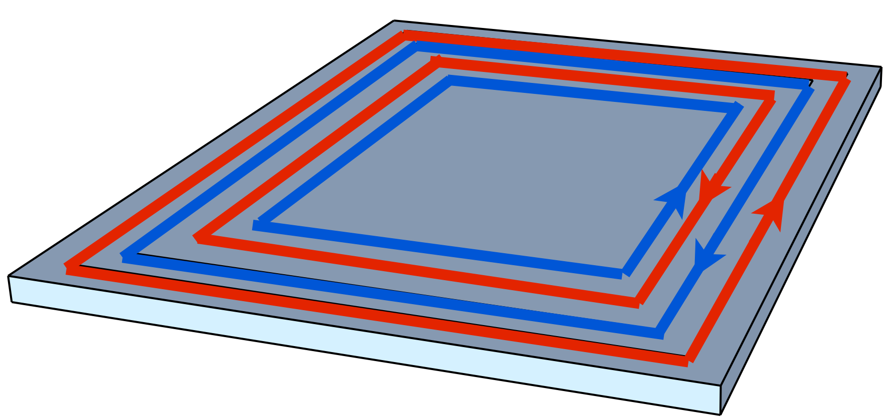


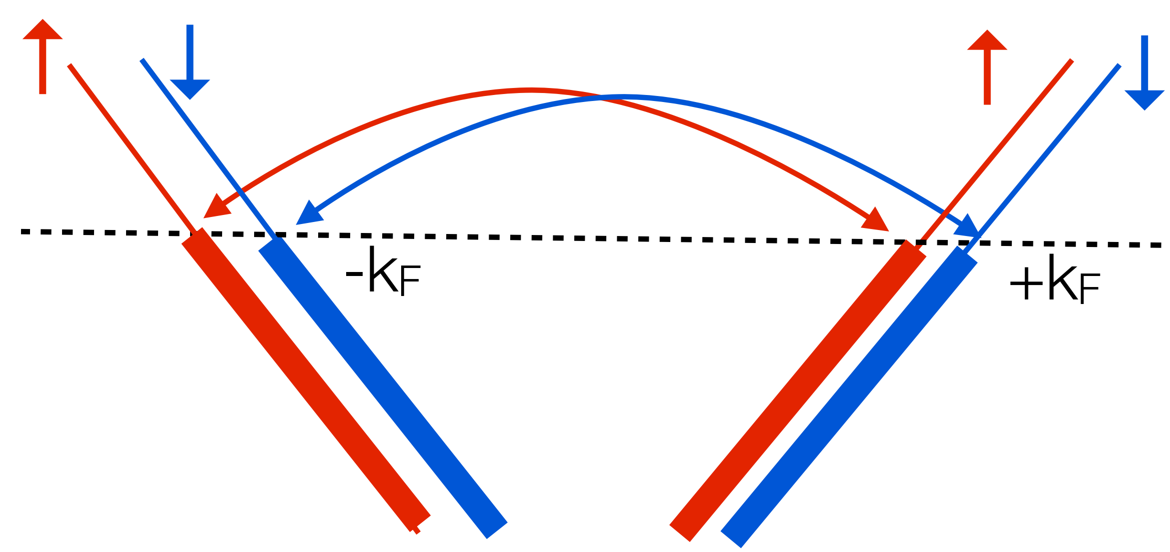


2 branches, but ≠ spins : no backscattering

⇒ topological order

with 4 modes :





Backscattering allowed ⇒ No topological order

Z_2 Topological index for QSHE : yes / no

Topological Invariance in 2D

C.L.Kane and E.J.Mele, PRL 95, 146802 (2005)

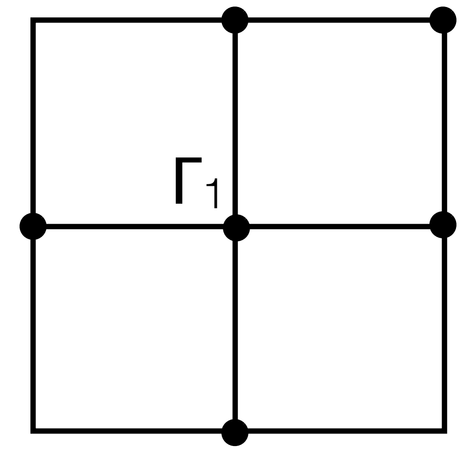
Time Reversal Symmetry : Θ antinunitary op. ($\langle \Theta\psi|\Theta\phi\rangle = \langle\phi|\psi\rangle$)

for spin 1/2 : $\Theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}$, $\Theta = e^{i\pi S_y} K$, $\Theta^2 = -1$

Kramers theorem : for time reversal invariant Hamiltonian ($[H,\Theta]=0$)

all eigenstates come (at least) by pairs of time reversed states

(otherwise $\Theta^2|u\rangle = |\lambda|^2|u\rangle$)



Simplest Case : only 2 energy bands $|u_{i=1,2}(\mathbf{k})\rangle$

Reciprocal Lattice Vectors $\mathbf{G} = n_1\mathbf{G}_1 + n_2\mathbf{G}_2$: represented on a square

4 Time-Reversal Invariant Momenta in the BZ : $\Gamma_{1\ldots4}$

(invariant by k →-k up to Bravais vector)

at Γ_i : $\Theta|u_j(\mathbf{\Gamma_i})\rangle$ equivalent to $|u_j(\mathbf{\Gamma_i})\rangle$ up to U(2) rotation

Focus on points $\mathbf{\Lambda}_m$ (if any) where $\Theta|u_j(\mathbf{\Lambda}_m\rangle$ is orthogonal to $|u_j(\mathbf{\Lambda}_m)\rangle$

$\mathbf{\Lambda}_m$ come by pair $(\mathbf{\Lambda}_m, -\mathbf{\Lambda}_m)$

2 pairs can annihilate each other by smooth deformation of $|u_{i=1,2}(\mathbf{k})\rangle$ by $\mathbf{\Lambda}_1 \to -\mathbf{\Lambda}_2)$

Single pair cannot annihilate (through Γ_1)

Parity of Number of pairs $(\mathbf{\Lambda}_m, -\mathbf{\Lambda}_m)$: topological invariant of $|u_{i=1,2}(\mathbf{k})\rangle$

(Twisted Real Fiber Bundle)

Topological Invariance in 2D

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Reciprocal Lattice Vectors **G** = (n_1**G**$_1$ + n_2**G**$_2$)/2 : represented on a square

4 Time-Reversal Invariant Momenta in the BZ : $\Gamma_{1...4}$

(invariant by k →-k up to Bravais vector)

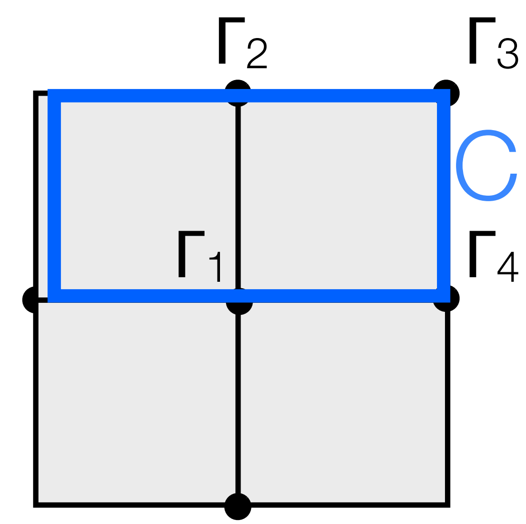
Consider the matrix $m_{ij} = \langle u_i(\mathbf{k})|\Theta|u_j(\mathbf{k})\rangle = \epsilon_{ij} P(\mathbf{k})$

P(**k**) : Pfaffian →generalization to higher number of bands

$|P(\mathbf{\Gamma_i})| = 1$ at TRIM $\Gamma_{1...4}$

Invariant Δ given by winding of phase of P(**k**) along path C

$$\Delta = \frac{1}{2\pi i}\oint_C d\mathbf{k}.\nabla_{\mathbf{k}} log(P(\mathbf{k}))$$



But not very practical...

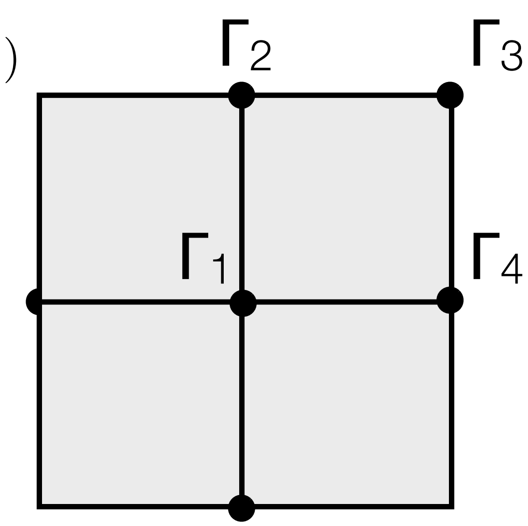
Topological Invariance in 2D

L. Fu and C.L.Kane, PRB 74, 195312 (2006)
L. Fu and C.L.Kane, PRB 76, 045302 (2007)

Previous definition : $m_{ij} = \langle u_i(\mathbf{k})|\Theta|u_j(\mathbf{k})\rangle$

$P(\mathbf{k}) = Pf(m_{ij})$

Top. Invariant Δ : winding of phase of P, $\Delta = \frac{1}{2\pi i}\oint_C d\mathbf{k}.\nabla_{\mathbf{k}} log(P(\mathbf{k}))$



Alternative definition : matrix $w_{ij} = \langle u_i(-\mathbf{k})|\Theta|u_j(\mathbf{k})\rangle$

w is unitary (|det w|=1)

w and m coincide at the TRIM $\Gamma_{1...4}$

$$(-1)^\Delta = \prod_{i=1}^{i=4} \frac{\sqrt{\det(w(\mathbf{\Gamma}_i))}}{\mathrm{Pf}(w(\mathbf{\Gamma}_i))}$$ where $\delta_i = \frac{\sqrt{\det(w(\mathbf{\Gamma}_i))}}{\mathrm{Pf}(w(\mathbf{\Gamma}_i))} = \pm 1$

With inversion symmetry : $\delta_i = \prod_{m=1}^{N} \xi_{2m}(\mathbf{\Gamma}_i)$ over 2N occupied bands

$\xi_{2m}(\mathbf{\Gamma}_i) := \pm 1$ Parity eigenvalue of **filled** band 2m

(and its Kramers degenerate 2m-1)

➠ Simple tool to look for topological nature of insulators

Topological Invariance : from 2D to 3D

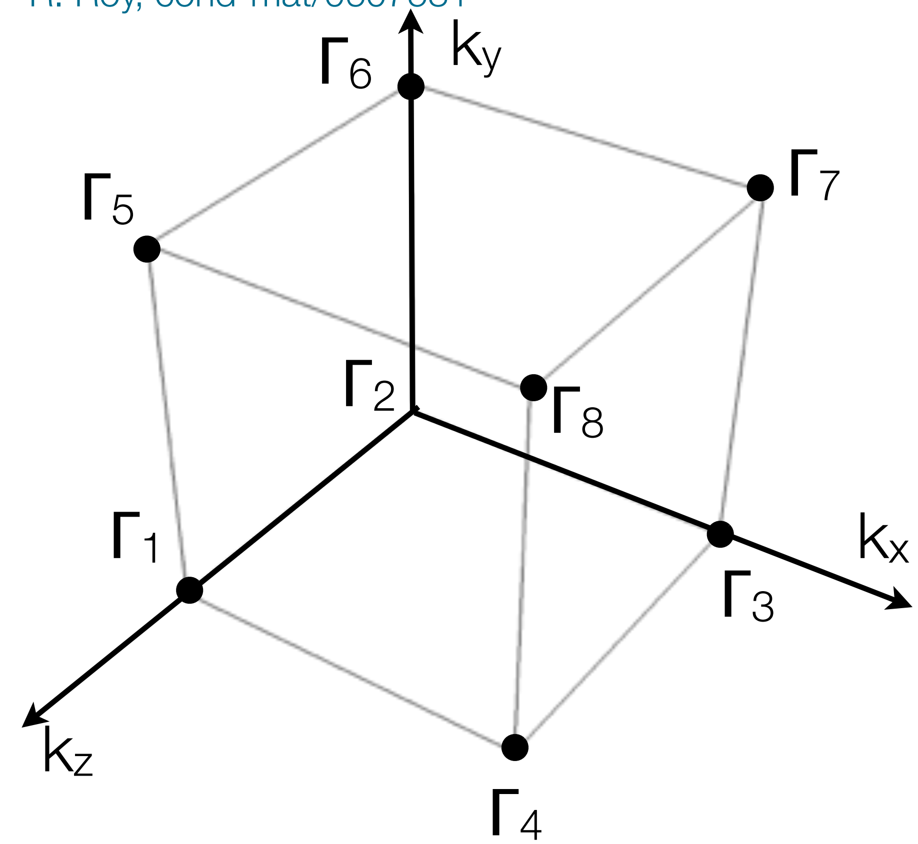
L. Fu, C.L.Kane, and E.J. Mele PRL 98, 106803 (2007)
J.E. Moore and L. Balents, PRB 75, 121306 (2007)
R. Roy, cond-mat/0607531

In 2D : $$(-1)^{\Delta} = \prod_{i=1}^{i=4} \frac{\sqrt{\det(w(\mathbf{\Gamma}_i))}}{\mathrm{Pf}(w(\mathbf{\Gamma}_i))}$$ with $w_{ij} = \langle u_i(-\mathbf{k})|\Theta|u_j(\mathbf{k})\rangle$

In 3D : 8 distincts TRIM $\Gamma_{1...8} = (n_1\mathbf{G}_1 + n_2\mathbf{G}_2 + n_3\mathbf{G}_3)/2$ $n_j = 0,1$

3 **G** dependant top. invariant : $(-1)^{\nu}_{i} = \prod_{\mathbf{\Gamma}_j/n_i=1} \frac{\sqrt{\det(w(\mathbf{\Gamma}_j))}}{\mathrm{Pf}(w(\mathbf{\Gamma}_j))}$

1 top. invariant : $$(-1)^{\nu_0} = \prod_{i=1}^{i=8} \frac{\sqrt{\det(w(\mathbf{\Gamma}_i))}}{\mathrm{Pf}(w(\mathbf{\Gamma}_i))}$$

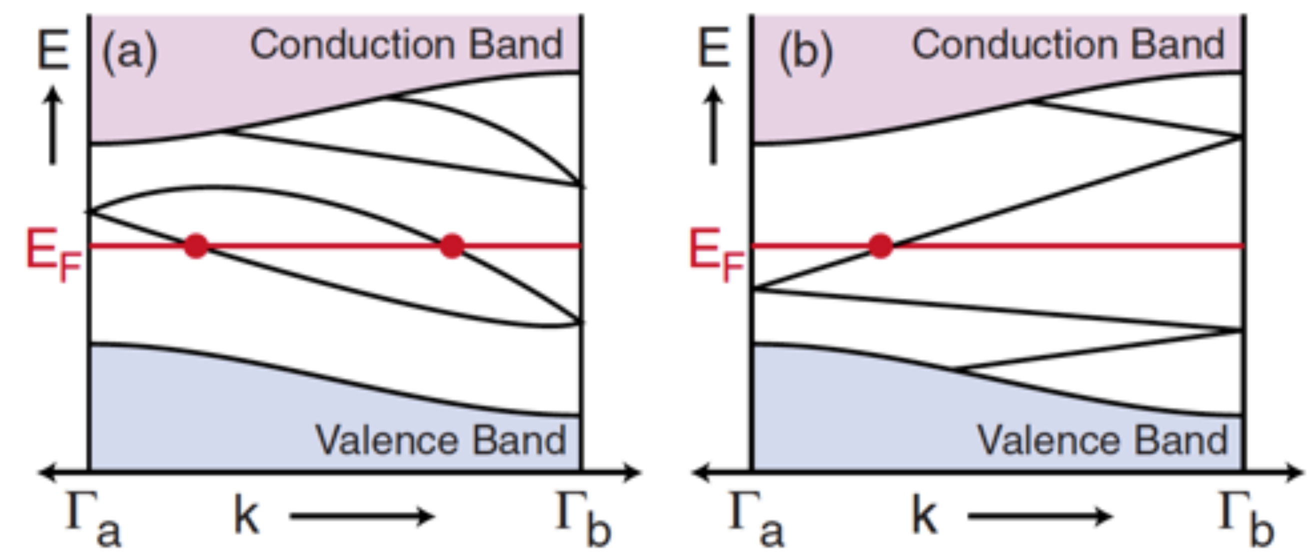


➠ Possible existence of 3D topological insulators

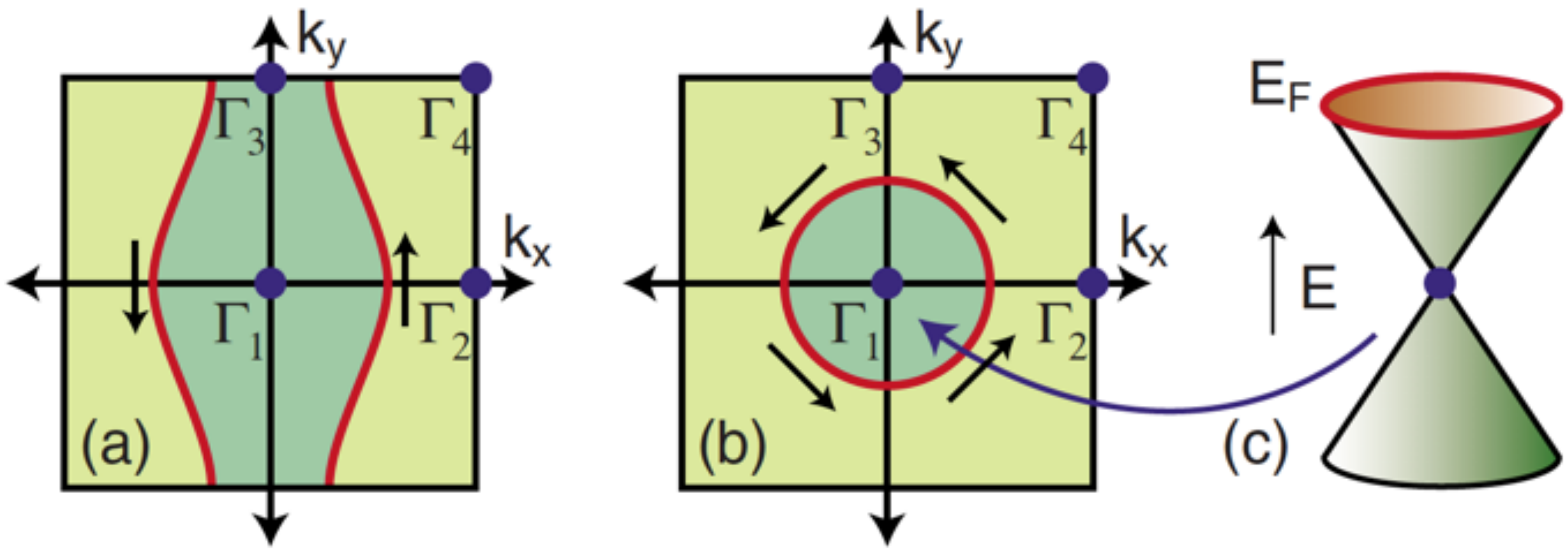
Topological Invariance from the edges

In 1D :
2 T-reversal symmetric momenta $\Gamma_a = 0$, $\Gamma_b = \pi/a$

invariants : Δ whether edge Fermi line cuts (odd times) the line $\Gamma_a \rightarrow \Gamma_b$



In 2D :
invariants : $\nu_{1..3}$ whether edge Fermi surface cuts (odd times) the line $\Gamma_1 \rightarrow \Gamma_b$
NEW invariant : ν_0 whether Fermi surface encloses an odd number of Γ_a



«weak» topological insulator, $\nu_0 = 0$ (layered 2D TI)

«strong» topological insulator, $\nu_0 = 1$, not layered

Topological Invariance from the edges

In 1D :
2 T-reversal symmetric momenta $\Gamma_a = 0$, $\Gamma_b = \pi/a$

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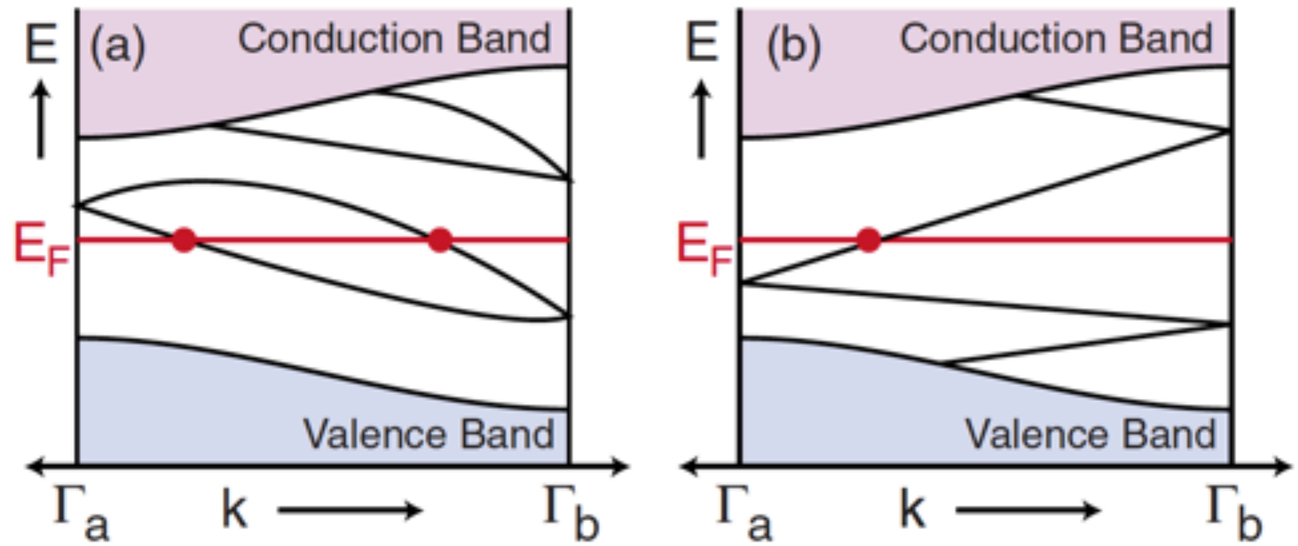

In 2D :
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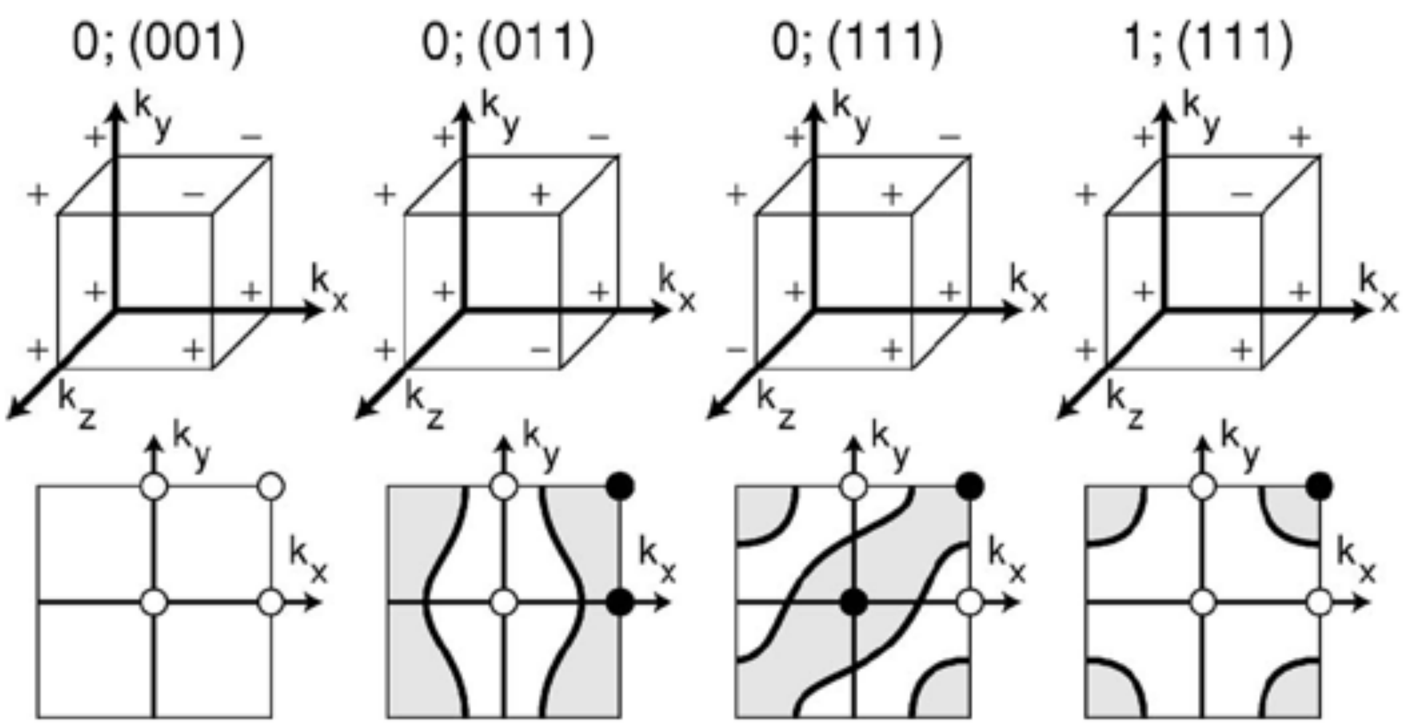
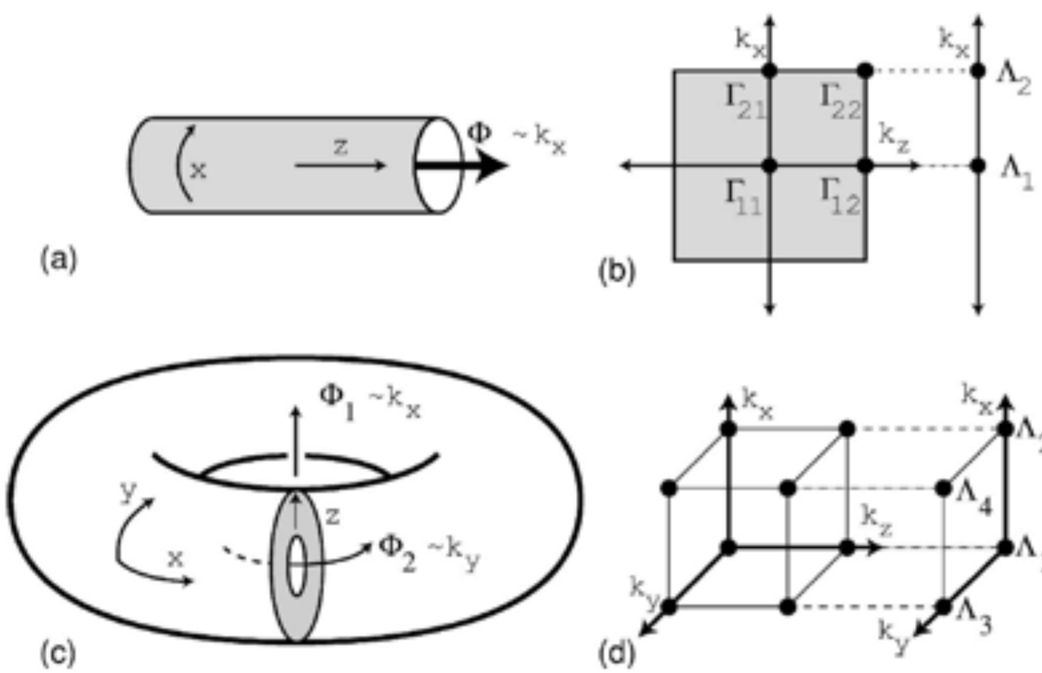
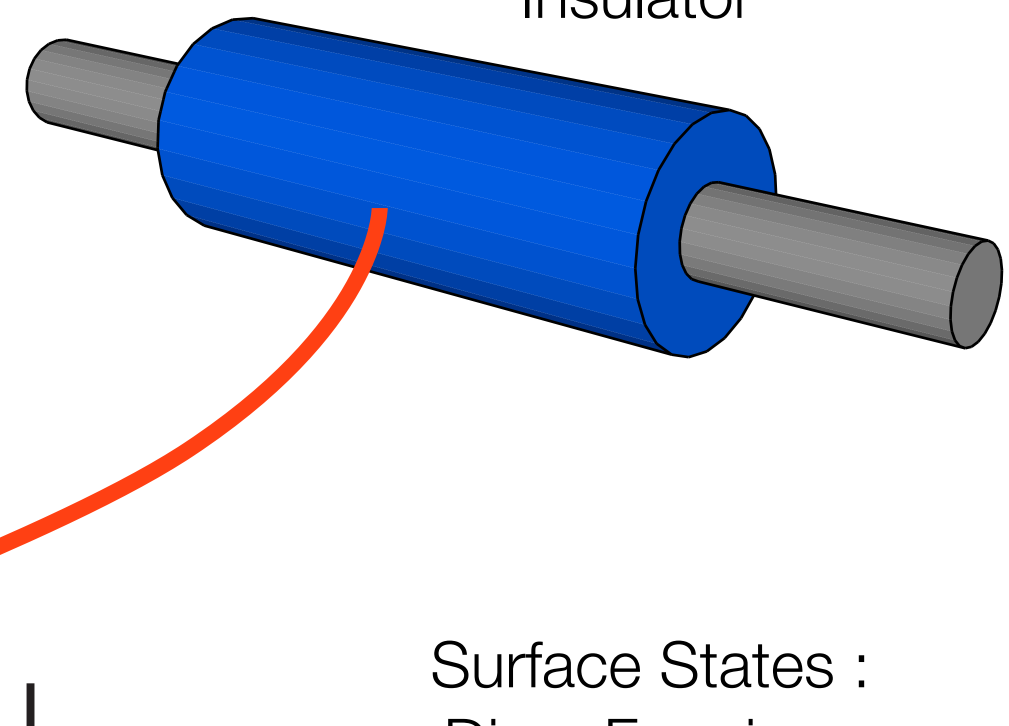
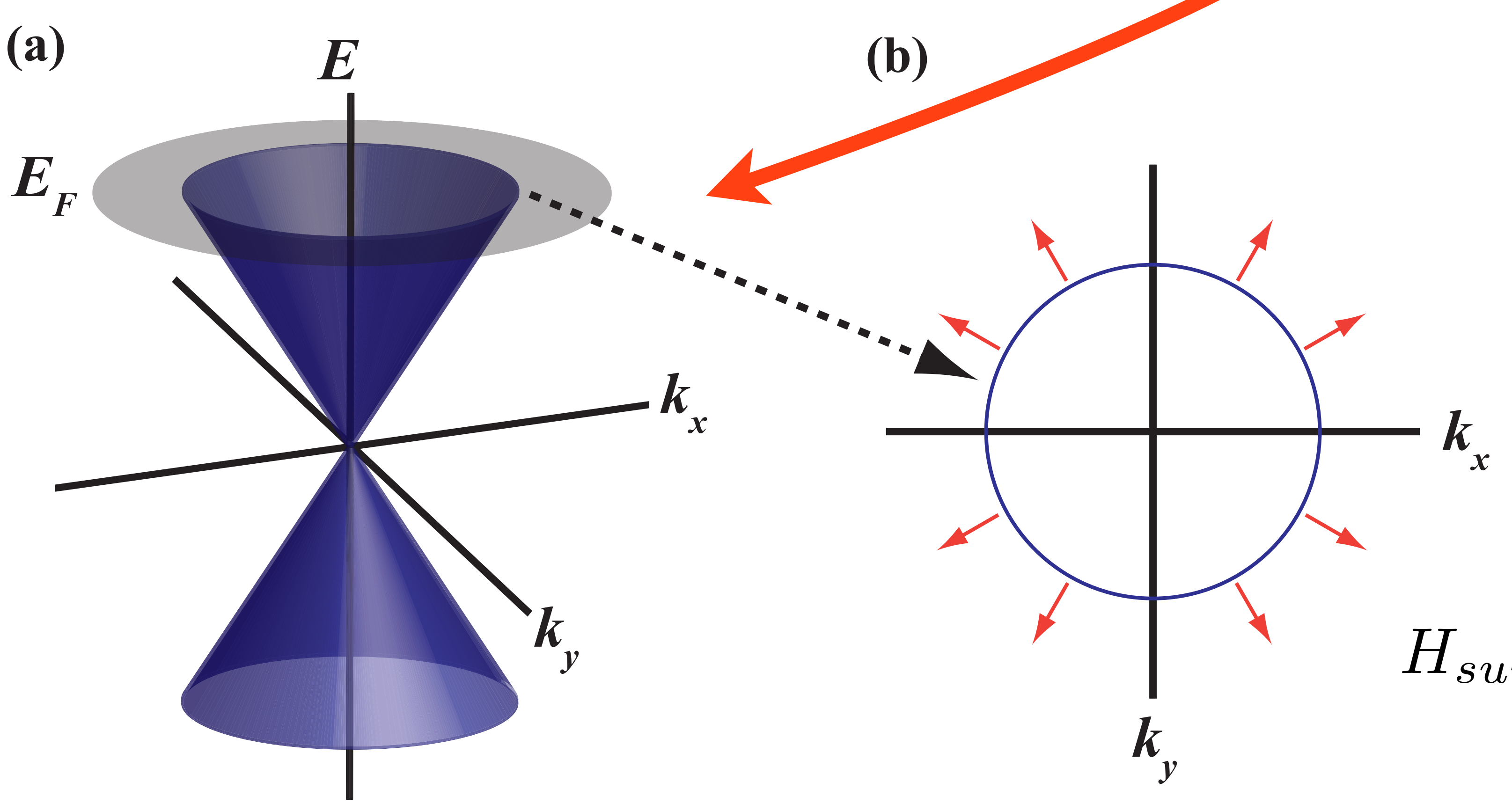




3D Topological Insulators

3D Topological Insulator





Surface States : Dirac Fermions

$$H_{surface} = -i\hbar v_F \; \sigma.\nabla$$

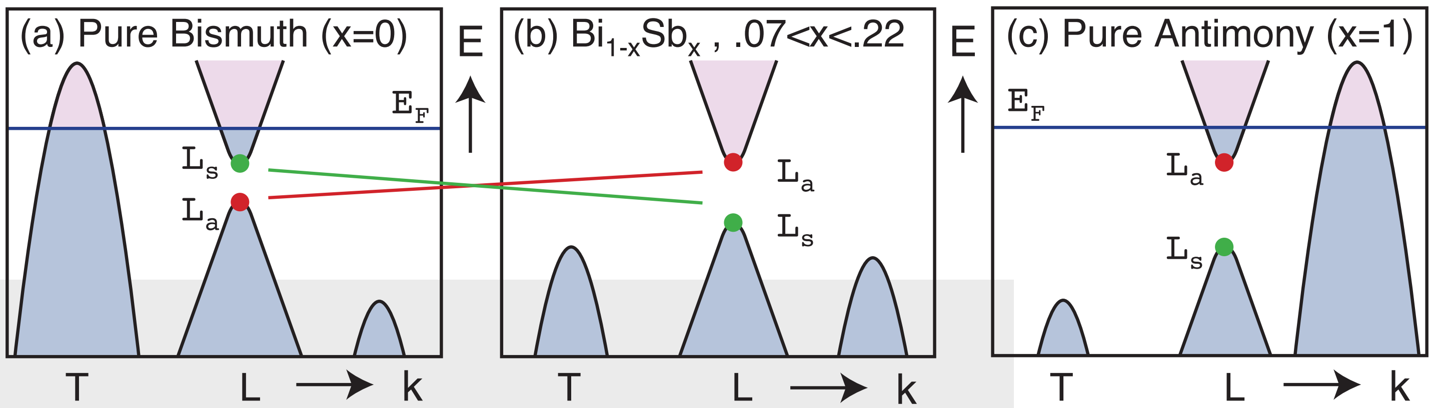
no violation of Fermion doubling theorem : 2nd cone is on the other side !

Topological Invariance and Band Inversion

With inversion symmetry : $\delta_i = \prod_{m=1}^{N} \xi_{2m}(\mathbf{\Gamma}_i)$ over 2N occupied bands

$\xi_{2m}(\mathbf{\Gamma}_i) = \pm 1$: Parity eigenvalue of **filled** band 2m

Topological Invariant : $(-1)^{\nu_0} = \prod_{i=1}^{i=8} \delta_i$



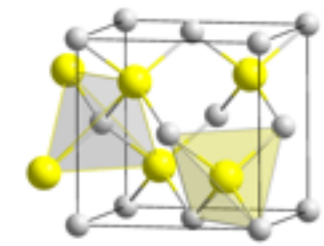
Most Insulator are trivial (not topological)

<u>General strategy in seeking topological insulators:</u>

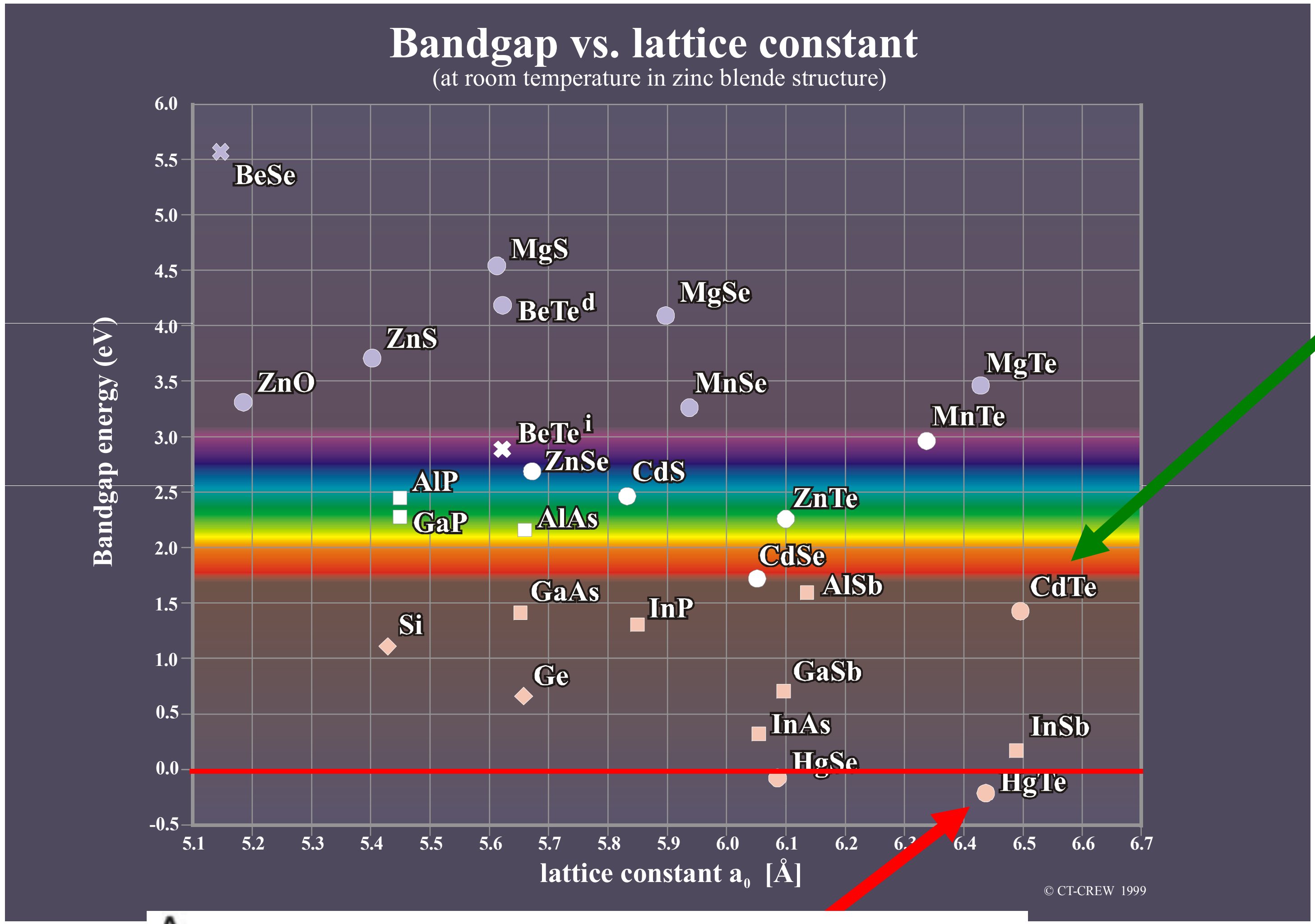
- find a compound with a band inversion with respect to known insulator, induced by strong spin orbit
- if inversion of bands with opposite parity eigenvalue : ν_0 will switch to non trivial value

➡ Candidate for Topological Insulators

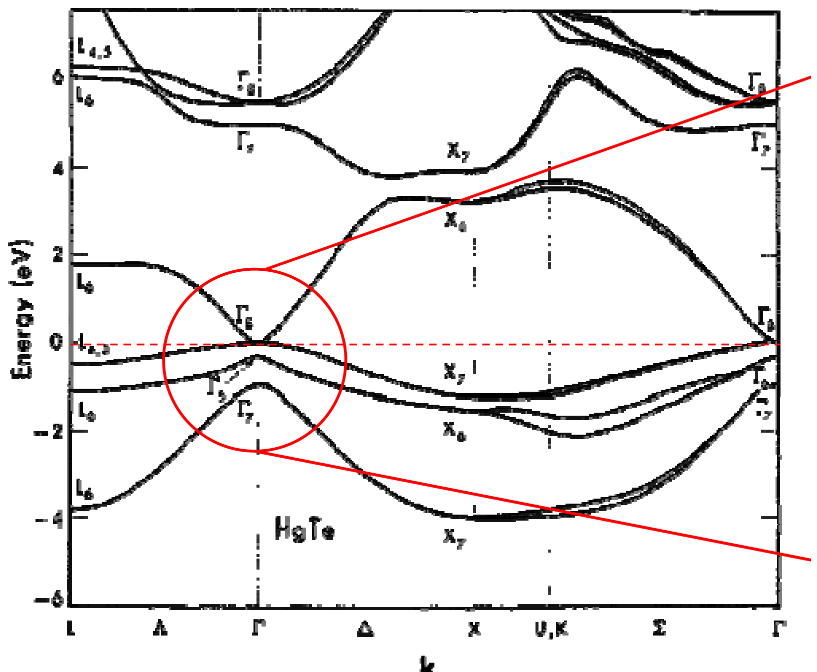
HgTe / CdTe Heterojunctions



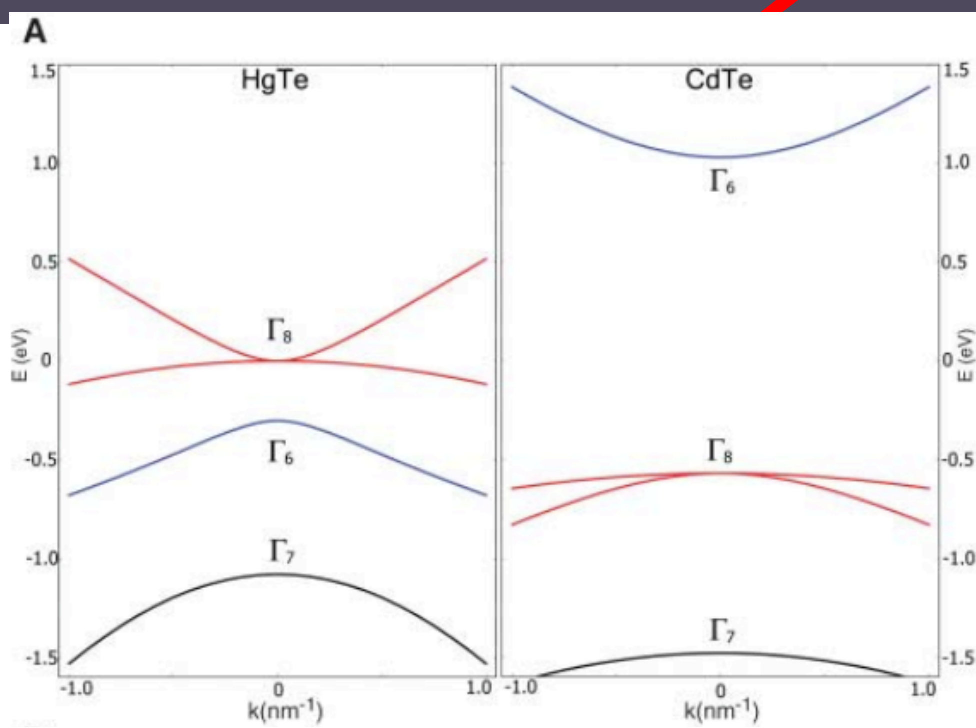
- Band Structure of HgTe : band inversion (strong spin-orbit)
- CdTe : no band inversion



HgTe band structure



D.J. Chadi et al. PRB, 3058 (1972)

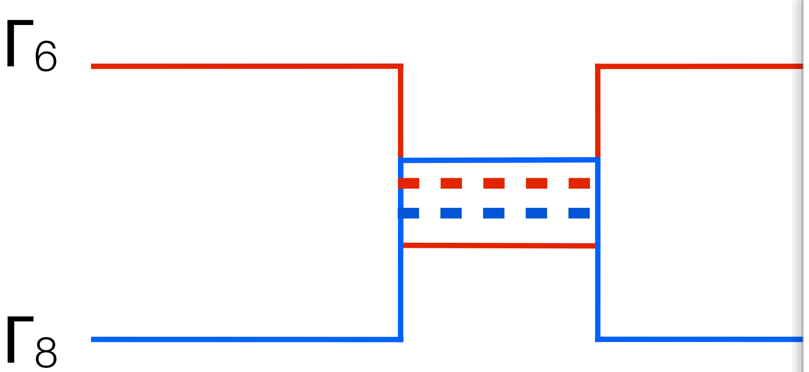


fundamental energy gap

$$E^{\Gamma 6} - E^{\Gamma 8} \approx -300\,\text{meV}$$

HgTe / CdTe Heterojunctions

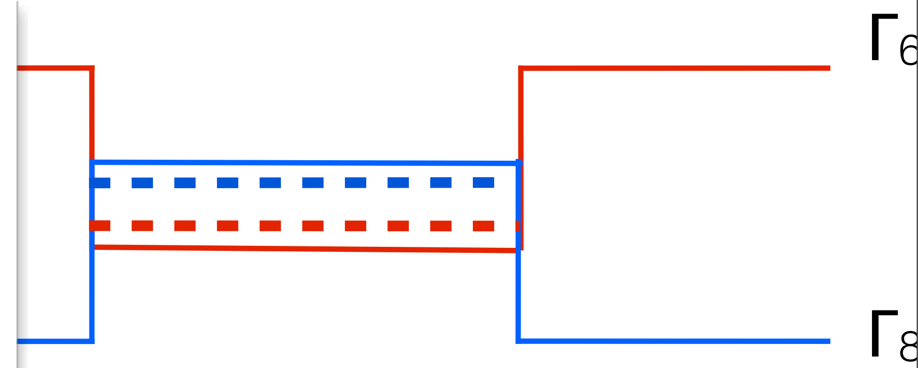
d<dc



d≈dc

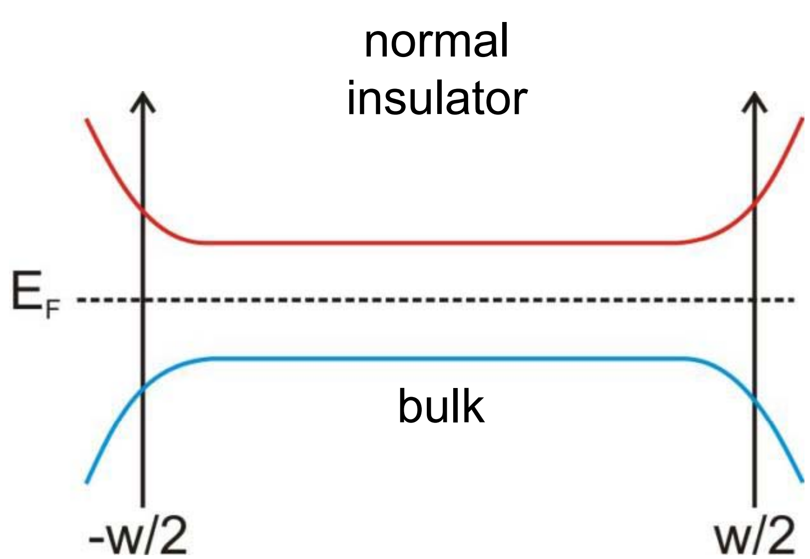
effective description :
Dirac model per spin
with m<0 or m>0

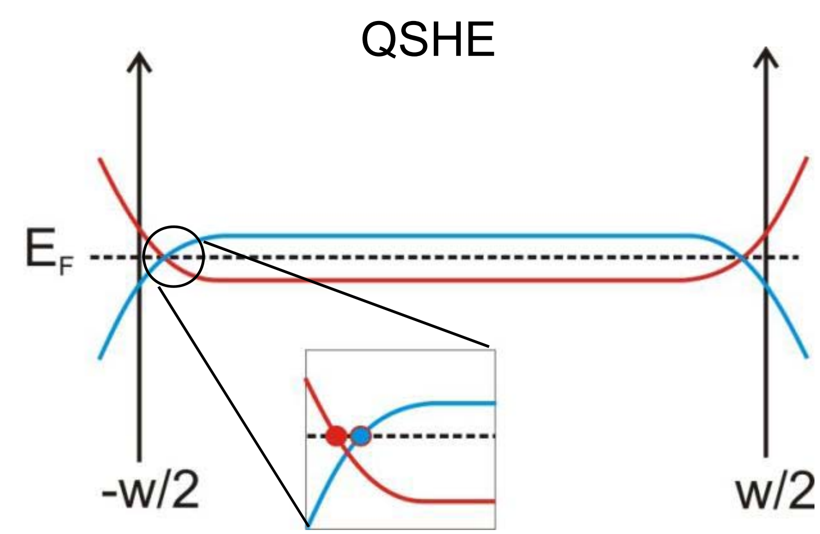
d>dc

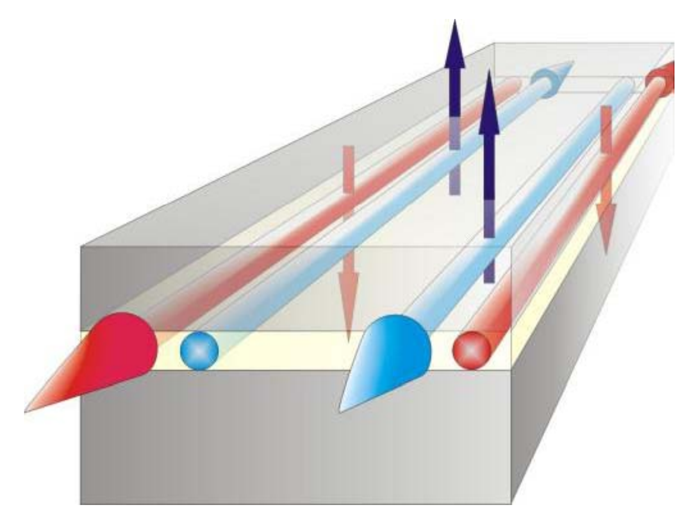


no band inversion in the junction

band inversion in the junction



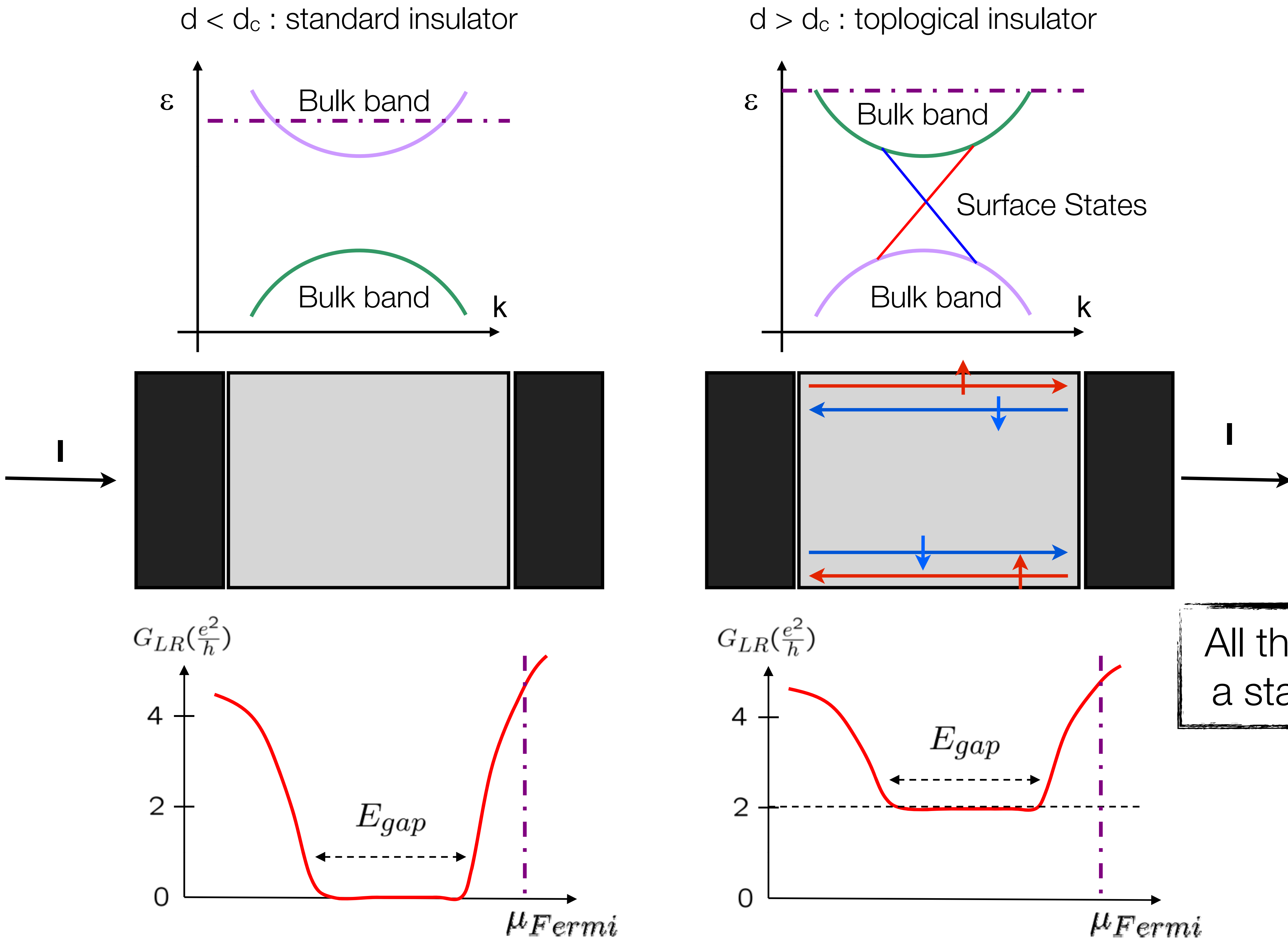




How to probe ? Conductance Measurements

König *et al.*, Science **318** (2007)

2 Terminal Conductance

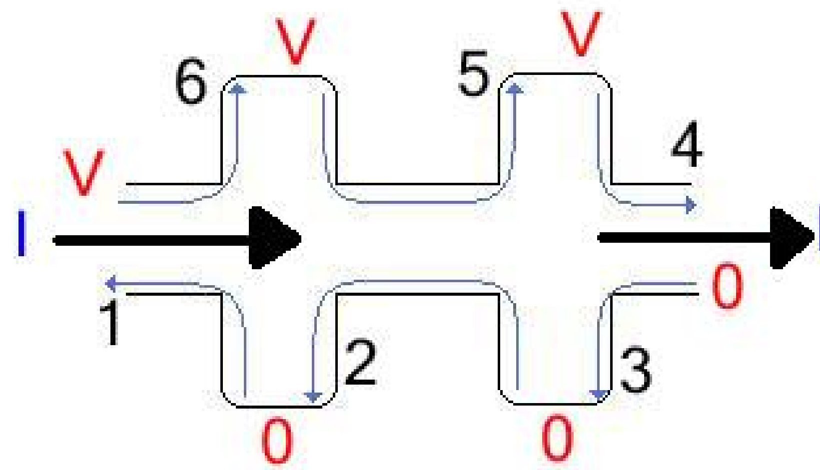


All the modes of a standard wire

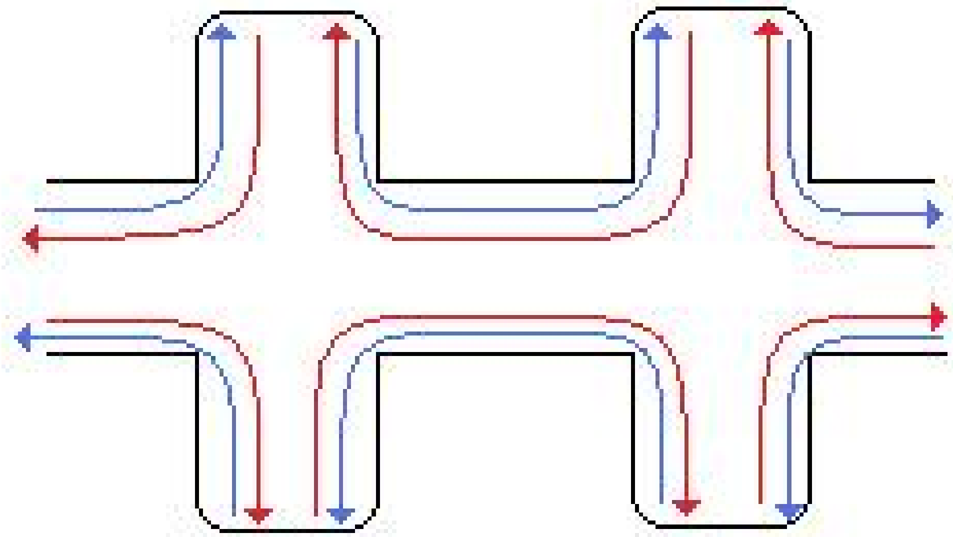
Beyond 2 terminals : Buttiker-Landauer descriprion

Roth *et al.*, Science **325** (2009)
P. Adroguer, D. Carpentier, *unpublished*

- Consider a Hall bar



$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \\ I_5 \\ I_6 \end{pmatrix} = \frac{e^2}{h} \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \\ \mu_6 \end{pmatrix}$$

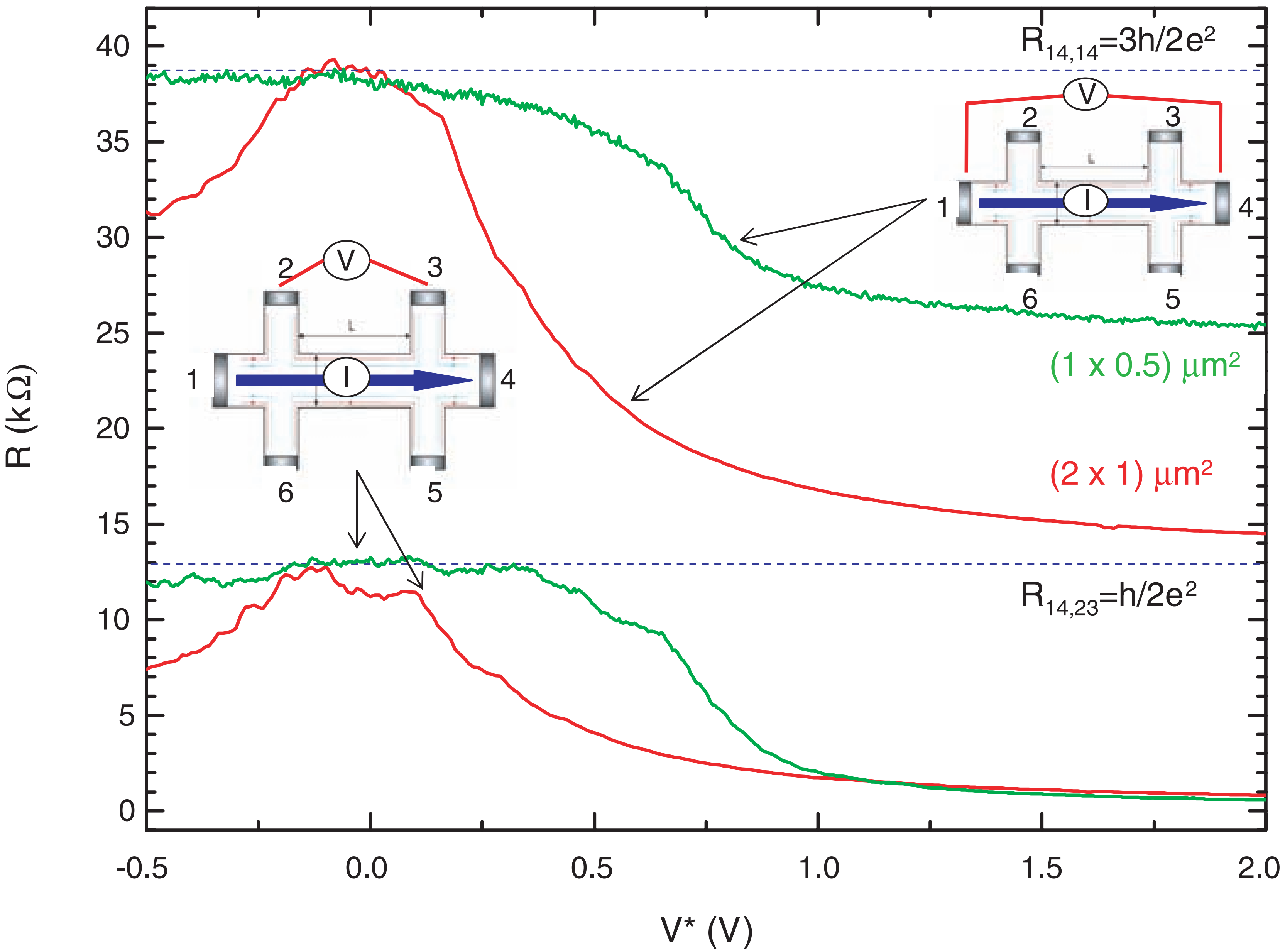


- Series of algebraic Conductance $G_{12,34}$, ...

Conductance Measurements

Roth et al., Science **325**, 294 (2009)

d=7,5nm > d_c=6,3nm
V* : gate voltage
T=10mK



Conductance Measurements

Roth et al., Science **325**, 294 (2009)

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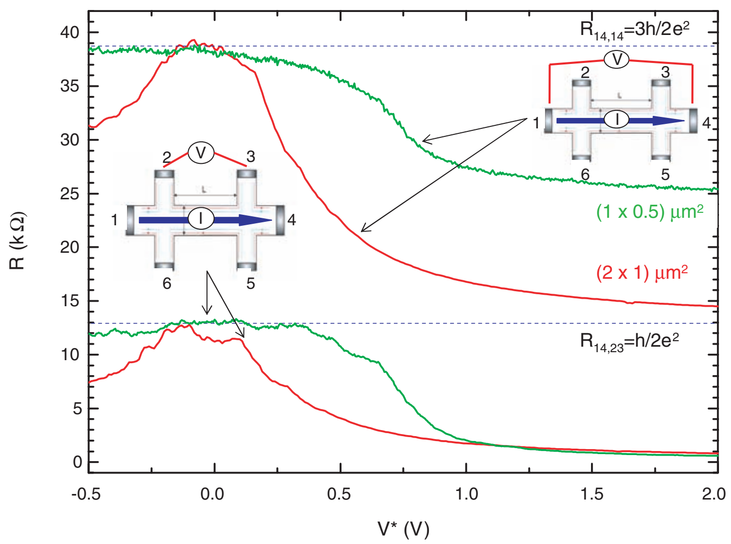
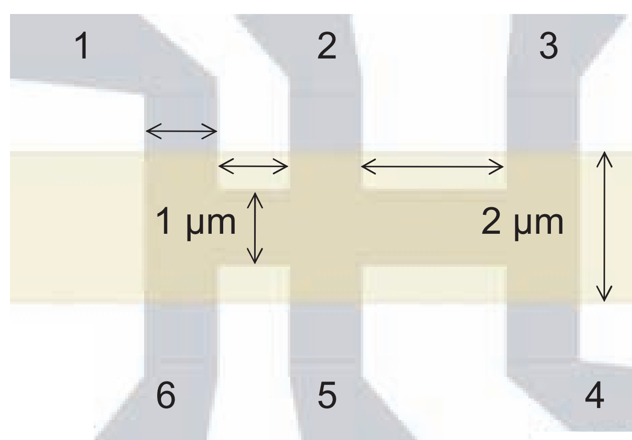
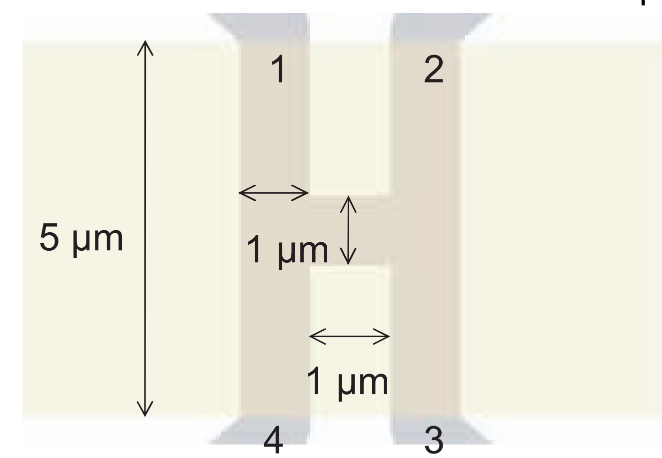


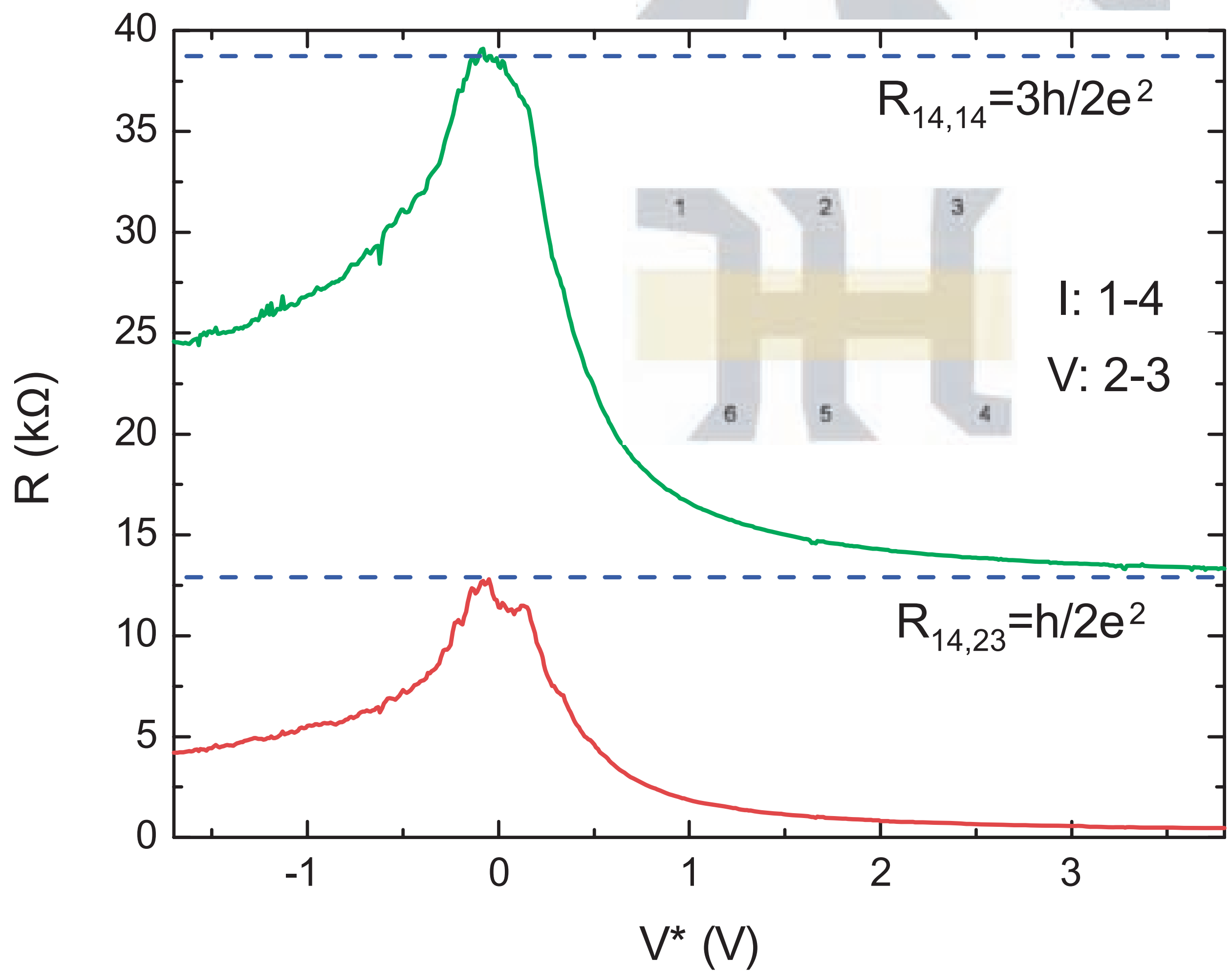
A



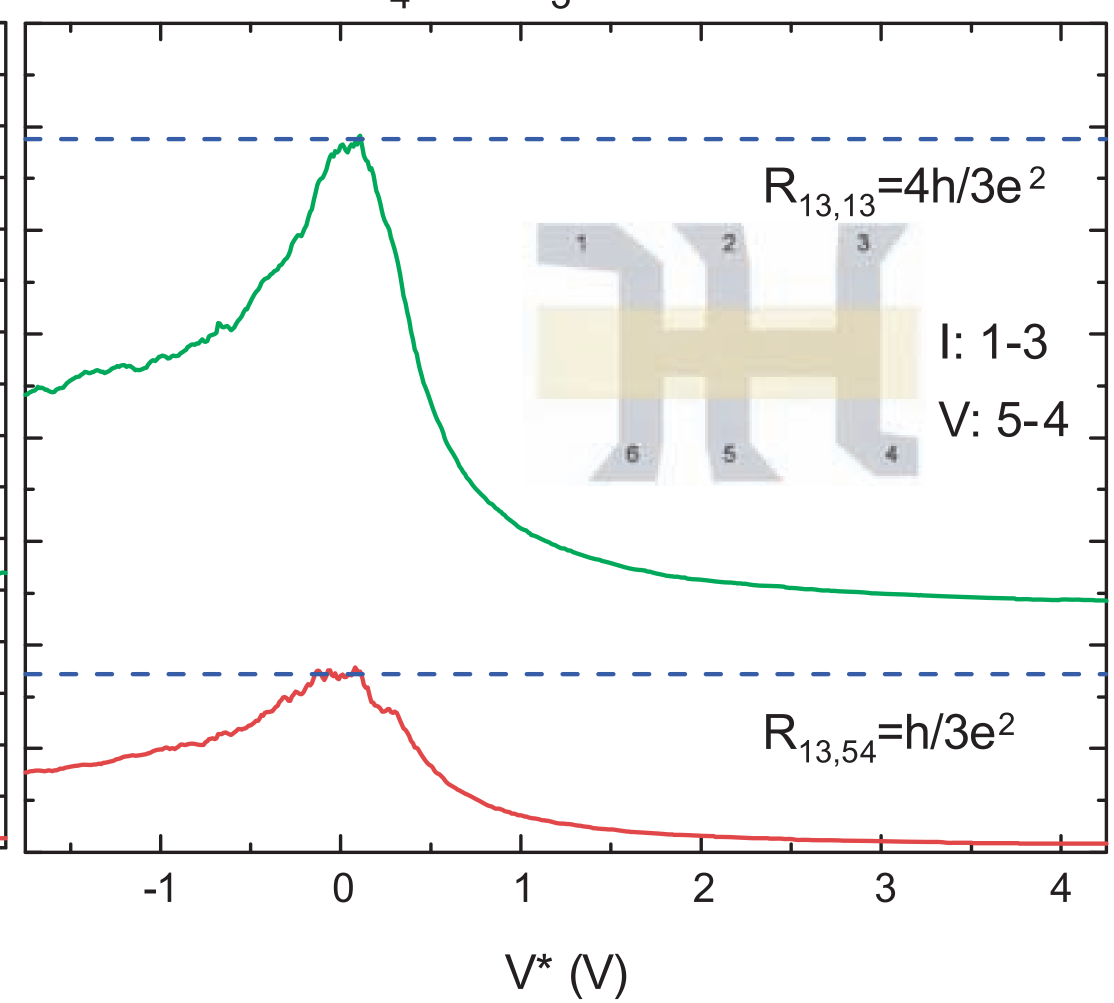
B



A

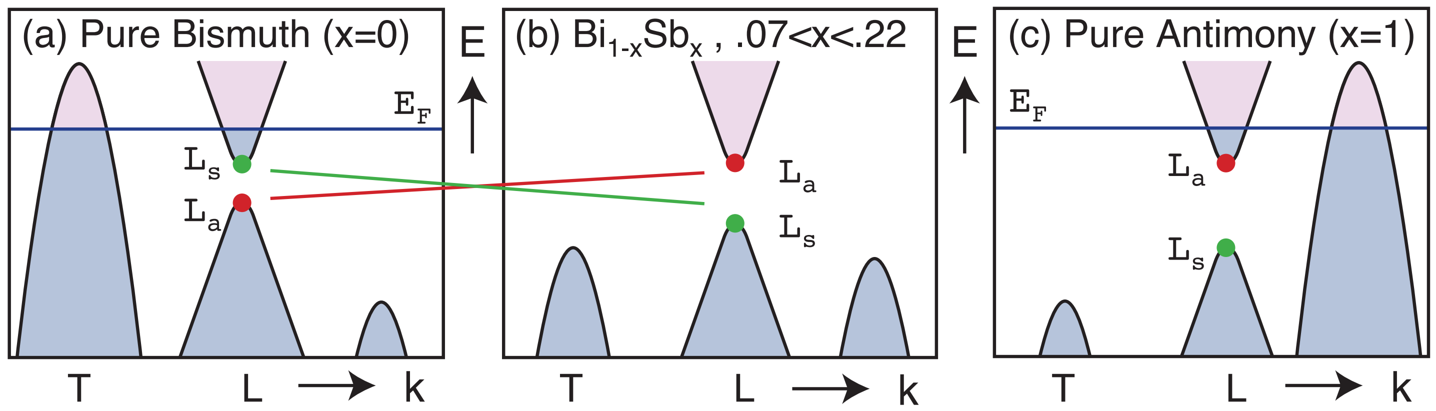


B



3D Topological Insulators

- First proposed candidate : $Bi_{1-x}Sb_x$
  again band inversion
  Fu and Kane PRB **76** (2007)



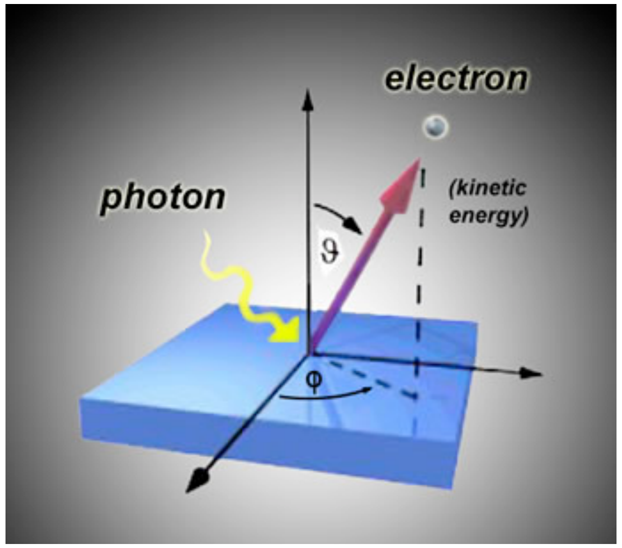
- Second generation 3D Topological Insulators : Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, ...
  Zhang H. et al., Nat. Phys. **5**, 438 (2009)

- Reference material : Bi_2Se_3
  - single Dirac cone at the surface
  - stoichiometric
  - large band gap : 0.3 eV (3600K)

How to probe experimentally ?

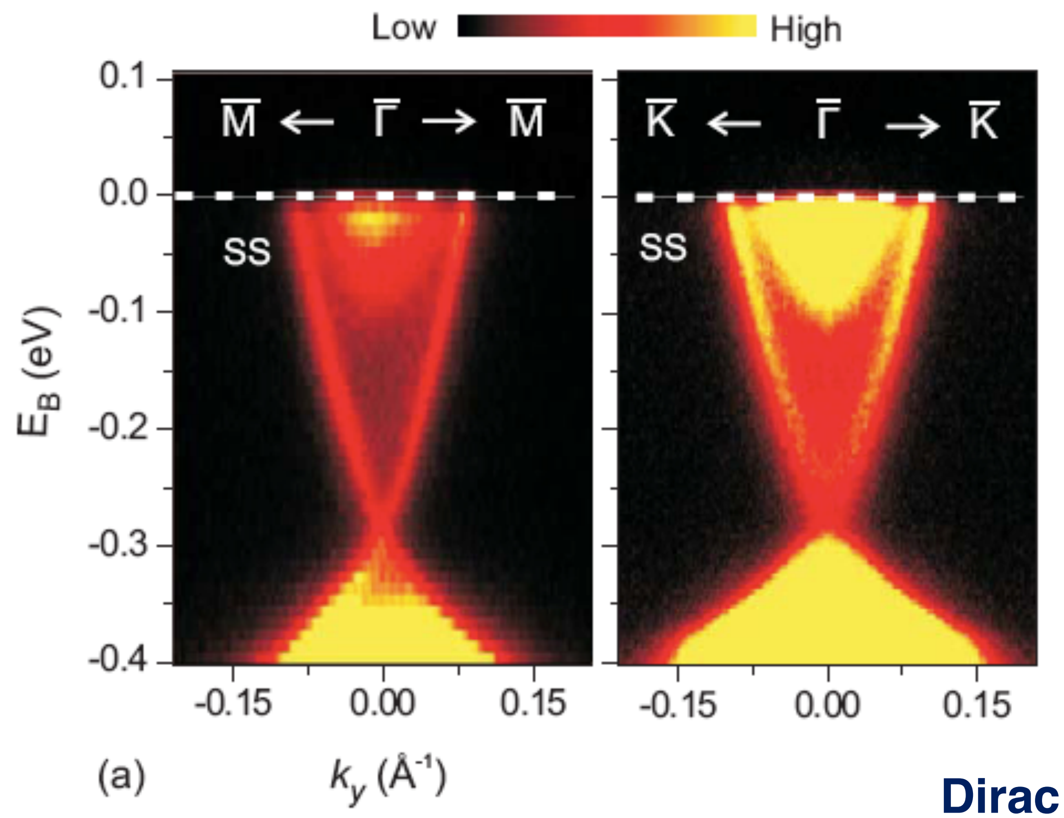
- existence of surface states : (spin resolved) ARPES Hasan's group (many papers)
- transport ... problematic Checkelsky *et al.*, PRL. **103**, 246601 (2009)

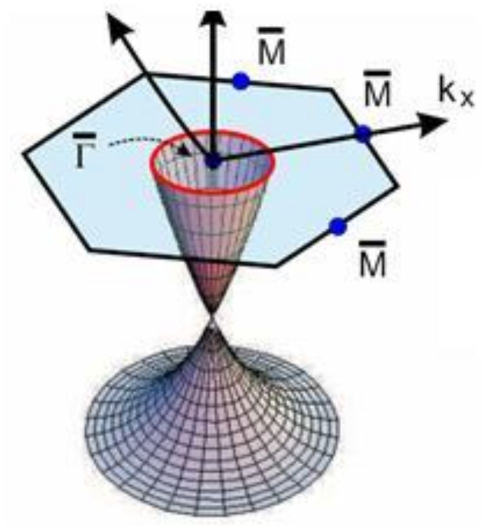
3D Topological Insulators : ARPES



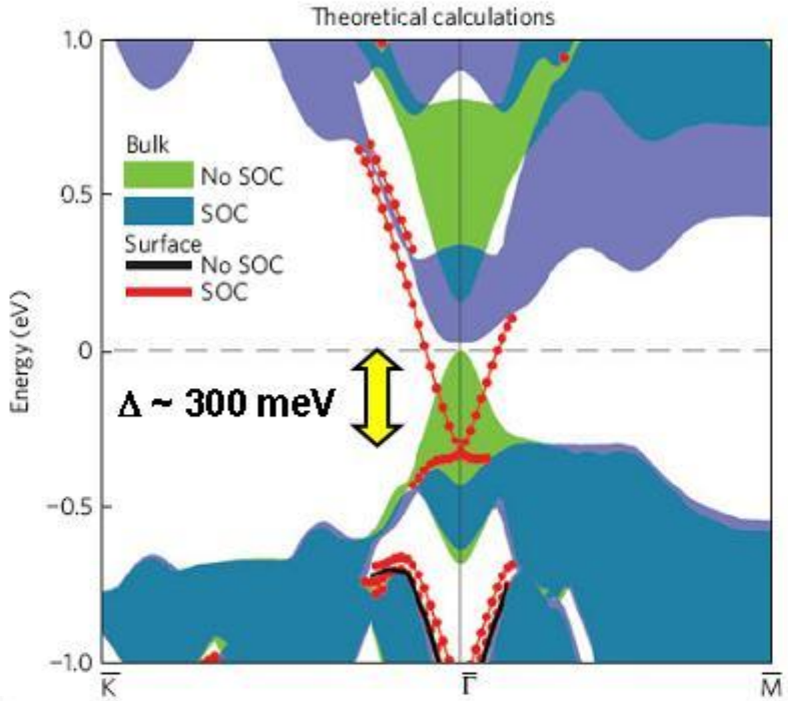
Measure Energy, momentum, and spin of surface electrons

- observation of Dirac cone in the bulk gap



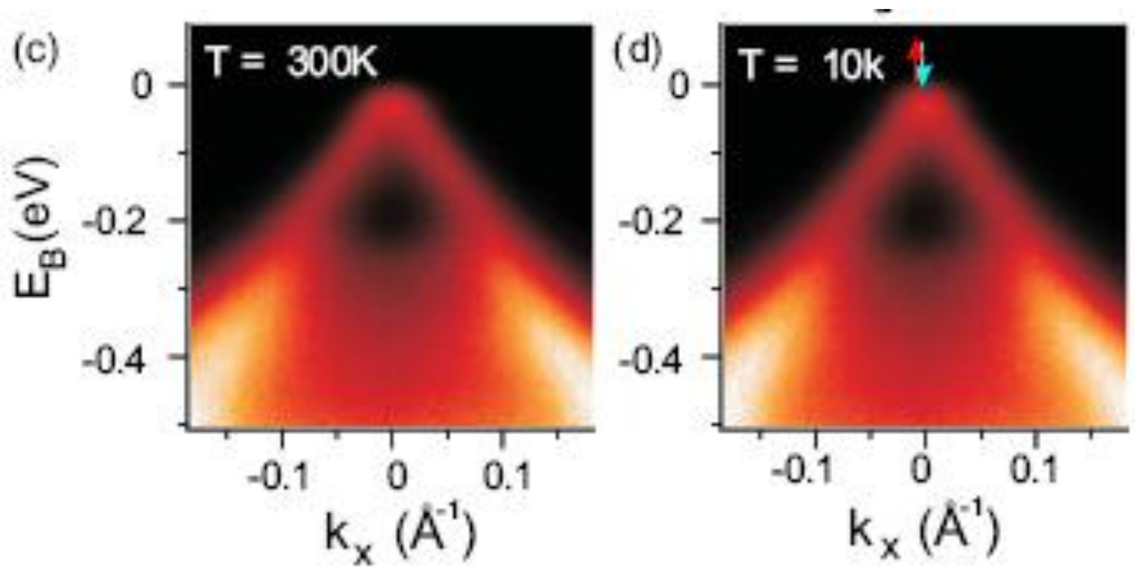


Bi_2Se_3



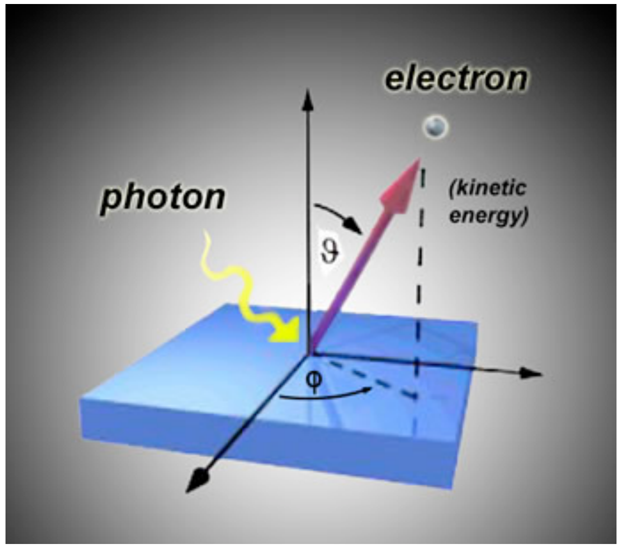
Dirac nodal Topo Insulator

- Stable up to room temperature

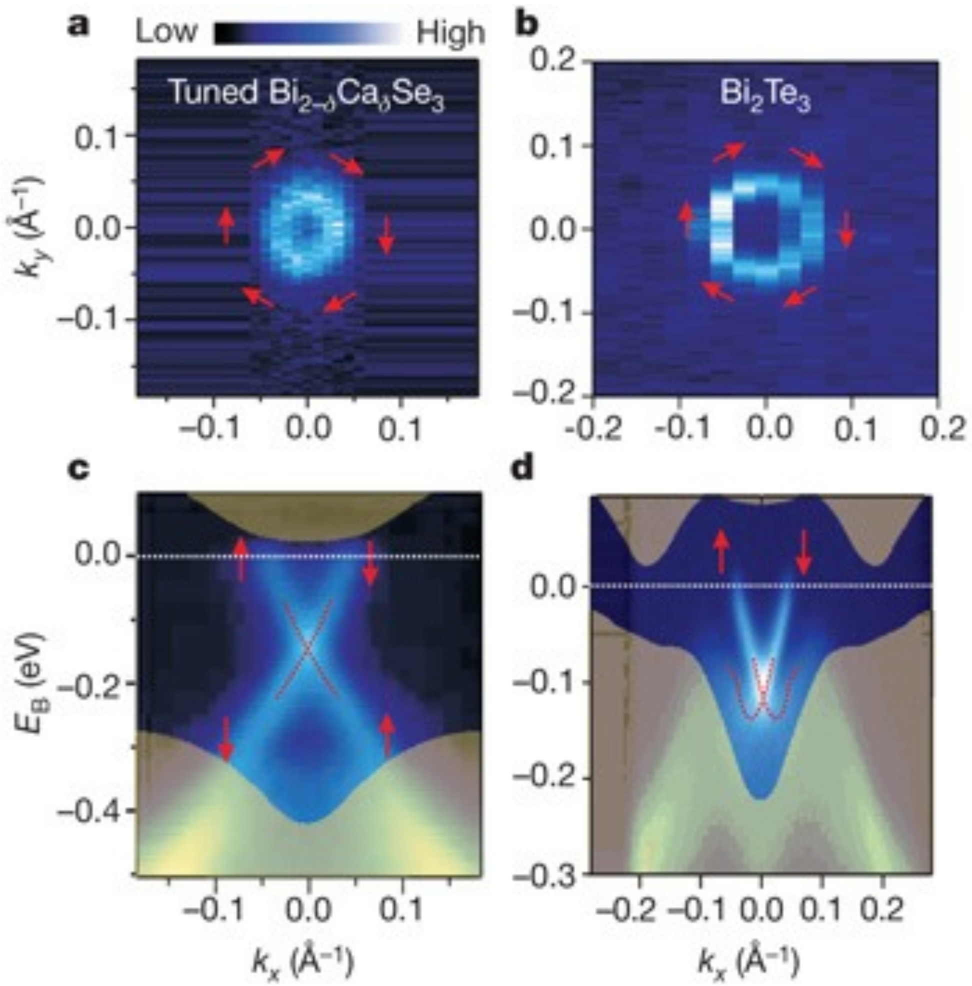


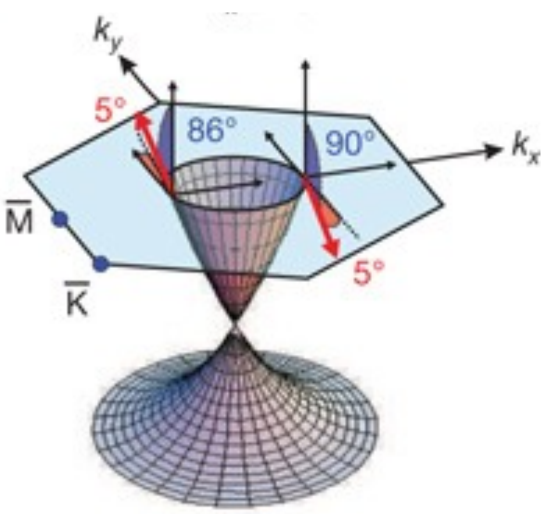
3D Topological Insulators : ARPES

Momentum - Spin locking : helical Dirac fermions



Hsieh *et al.*, Nature **460**, 1101 (2009)

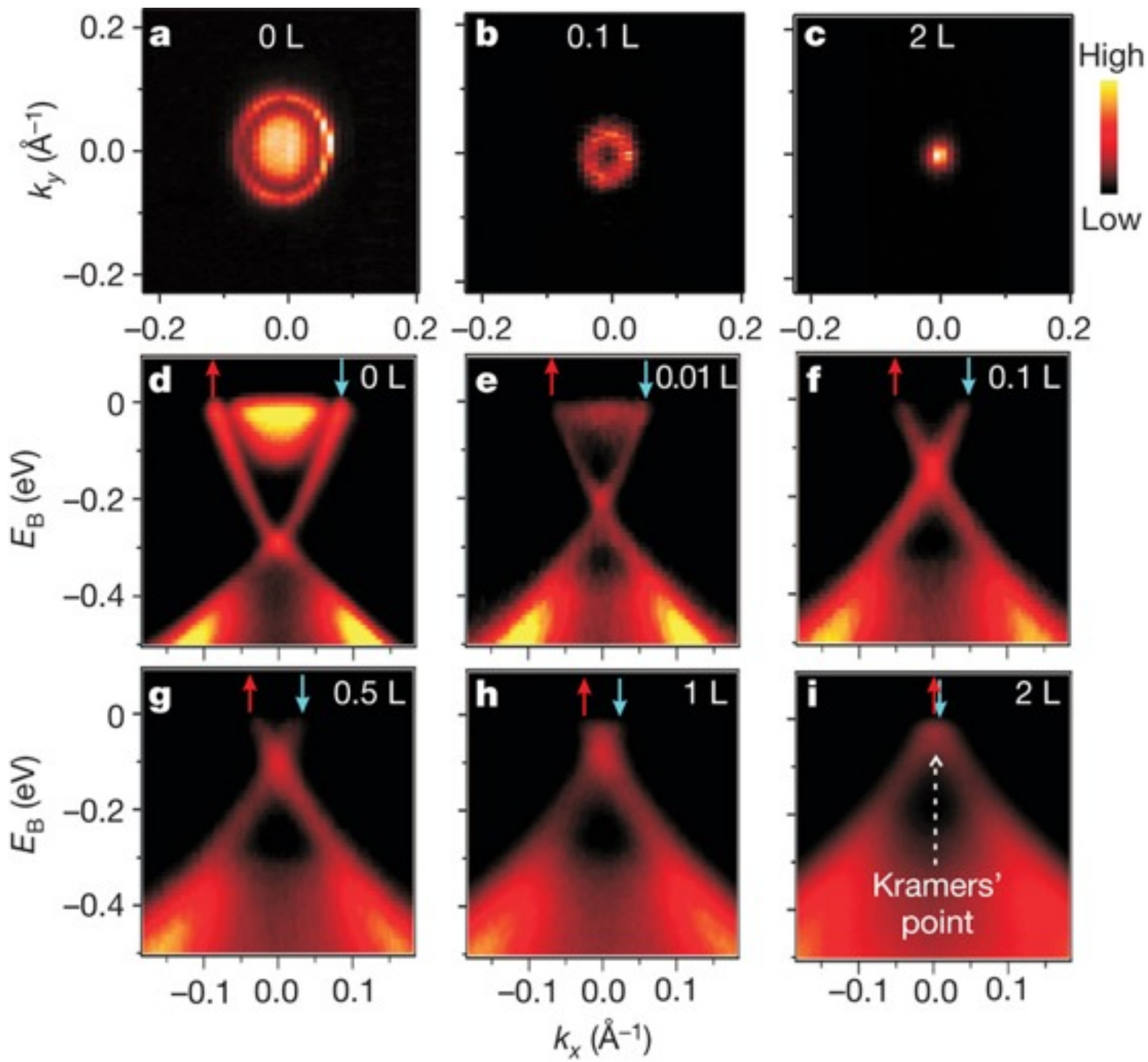


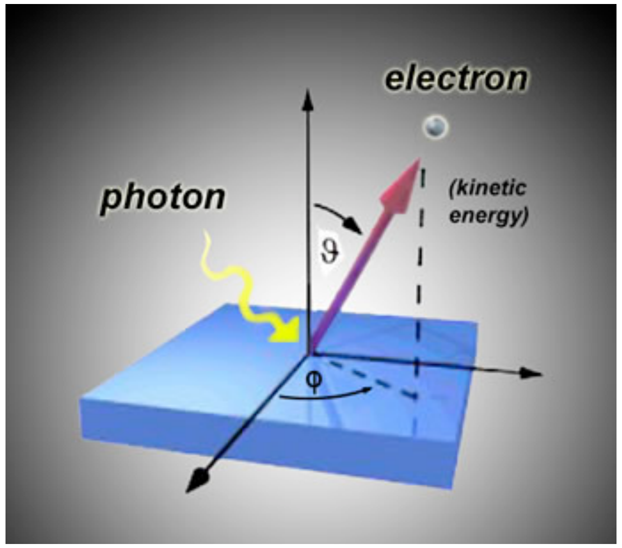


- Ca bulk doping

3D Topological Insulators : ARPES

Surface doping by NO_2 adsorption (hole doping)

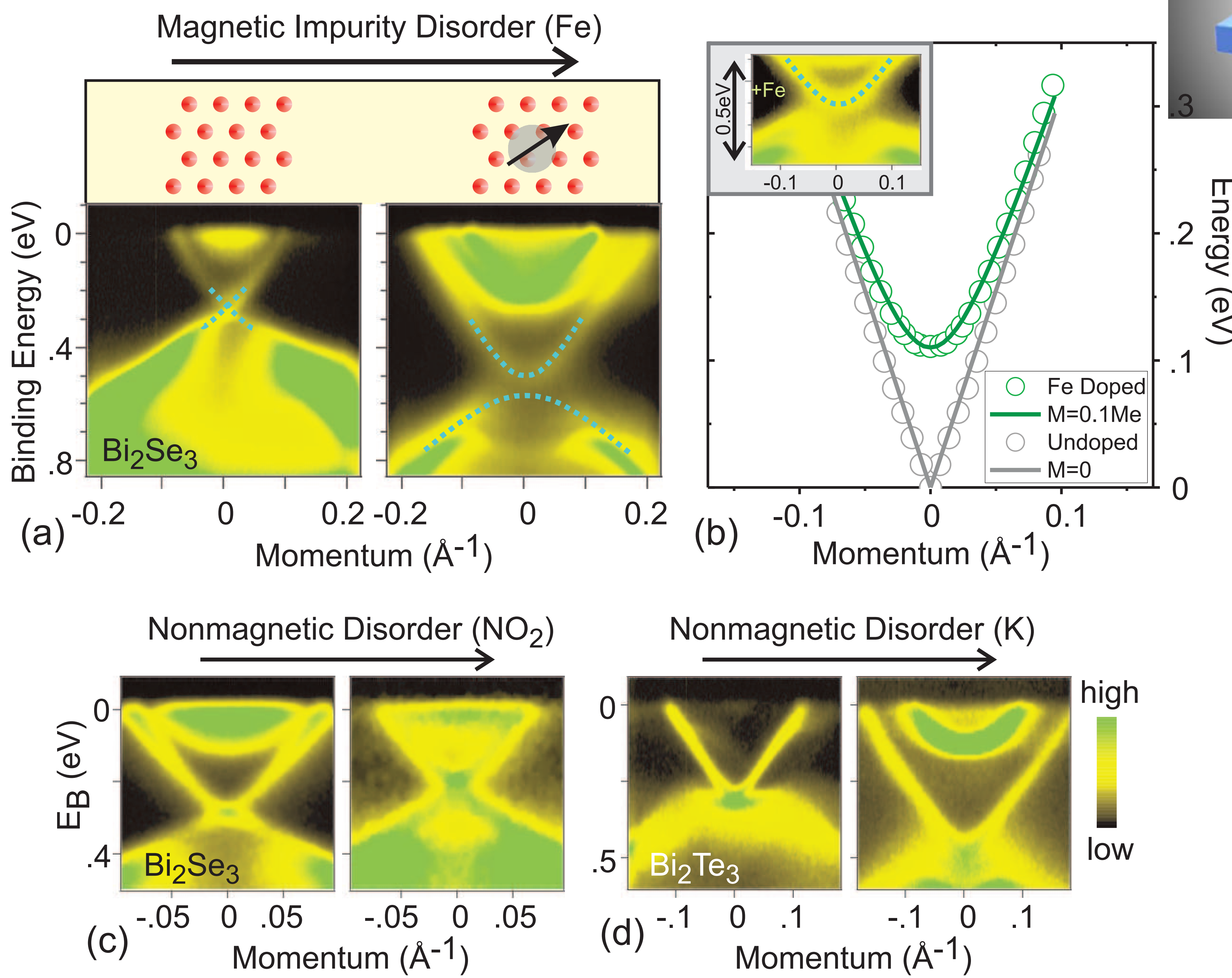


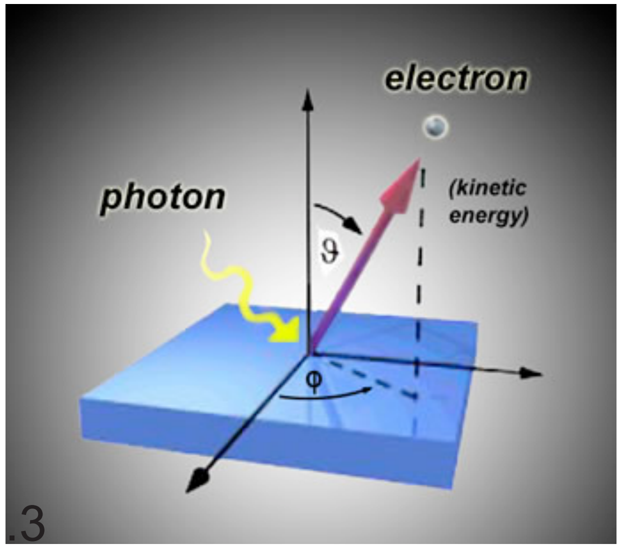


Hsieh *et al.*, Nature **460**, 1101 (2009)

3D Topological Insulators : ARPES

Magnetic impurities open a gap for the surface states





Xia *et al.* Nat. Physics **5**, 398 (2009)
Hsieh *et al.*, Nature **460**, 1101 (2009)

Transport measurement on Bi_2Se_3

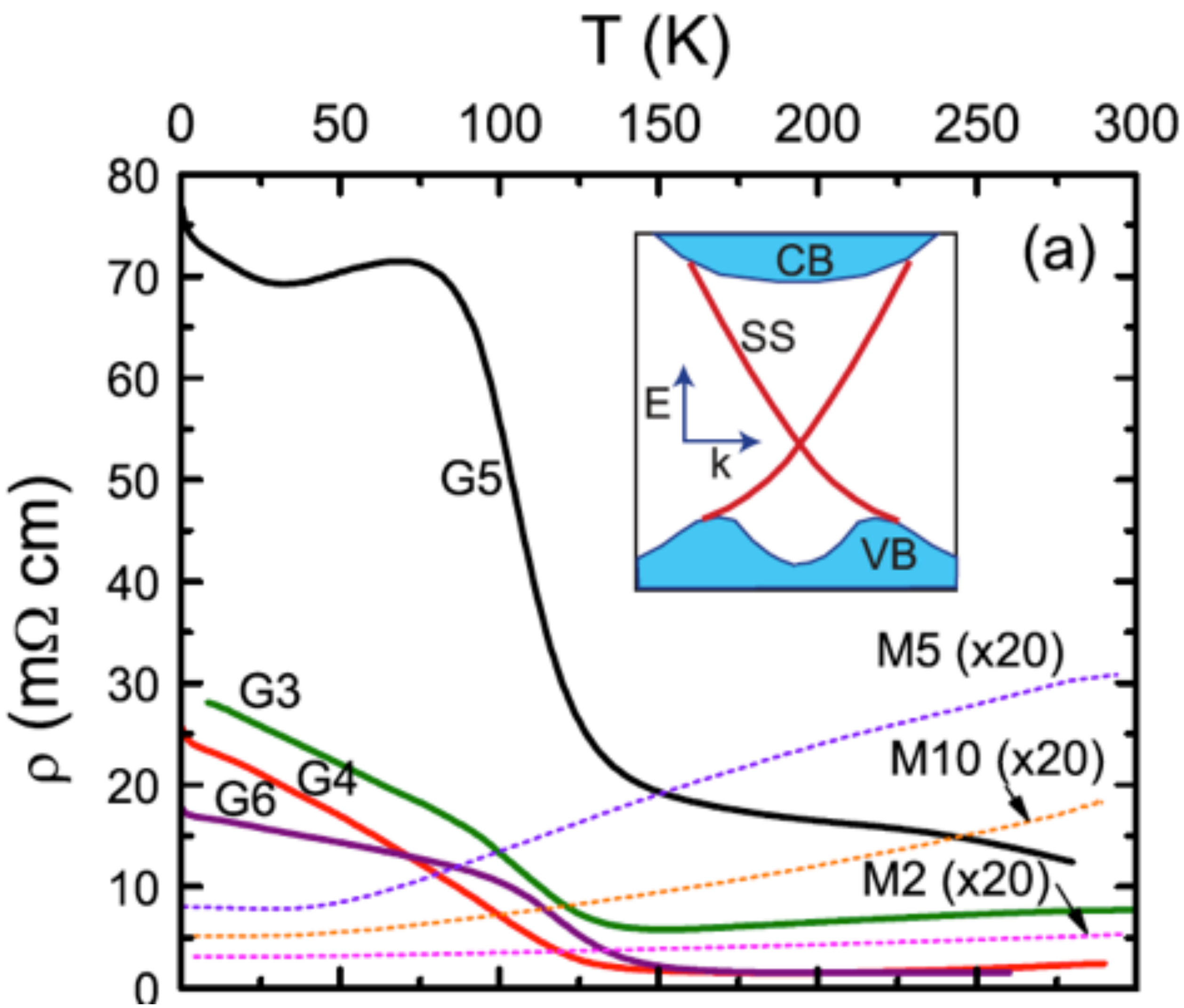
Checkelsky et al. PRL, 103 (2010)

Bi_2Se_3 : good candidate

- Large band gap : 300 meV
- Single Dirac surface state

... but metal ! ... μ_b in the conduction band

- chemical doping by Ca : $Ca_xBi_{2-x}Se_3$
- Residual transport by bulk states ?



Undoped versus doped samples
Various Ca doping

bulk sample (2x2x0.05 mm)

New materials : ternary compounds

Half Heusler semiconducting compounds :

Lin *et al.*, Nature Materials **9**, 546 (2010)

Chadov *et al.*, Nature Materials **9**, 541 (2010)

(X_2YZ or XYZ composition with X, Y the transition or rare-earth metals and Z the main-group element)

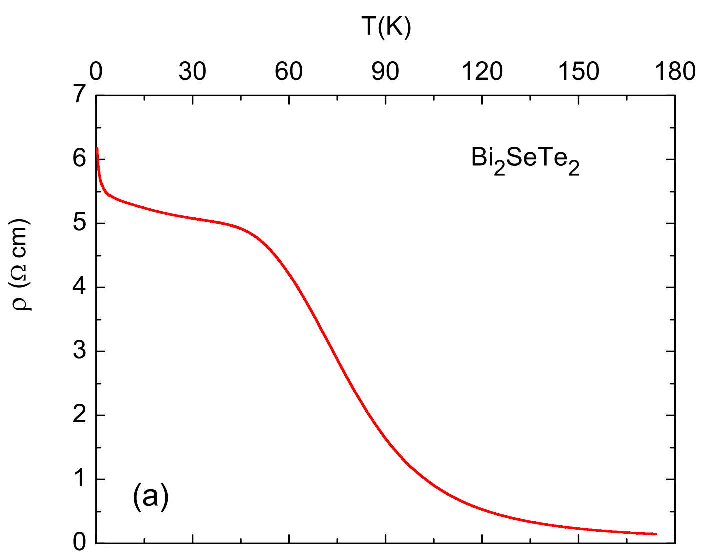
- band inversion found in ab initio studies for lots of them
- topological insulators coexisting with other order
  - LnPtBi (Ln=Nd, Sm, Gd, Tb, Dy) : TI + magnetism
  - YbPtBi : heavy fermion TI : topological Kondo insulator (???)
  - LaPtBi : TI + superconductivity (?)
- Problem : not insulators ...

Bi_2Te_2Se :

Z. Ren *et al.*, arxiv:1011.2846

J. Xiong *et al.*, arxiv:1101.1315

- Topological insulator with large bulk resistivity (6 Ωcm at 4 K)
- Signature (SdH oscillations) of metallic edge transport with high mobility (μ_s ~ 2,800 cm^2/Vs)



The forgotten subjects ...

- Anomalous axion electrodynamics

  Qi, Hughes and Zhang, PRB **78** (2008)
  Essin, Moore and Vanderbilt, PRL **102**, 146805 (2009)

- Classifications of topological insulators / superconductors : the 10-fold way, via study of disorder effect (Non Linear Sigma)

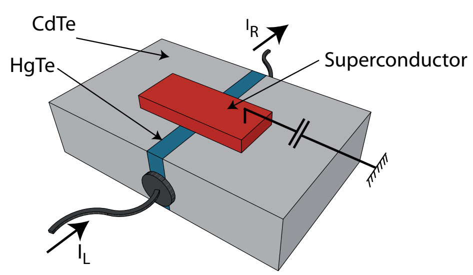
  Schynder et al., PRB **78** (2008)
  Kitaev, AIP Conf. Proc. **1134**, 22 (2009)

- the quest for Majorana fermions at Topological Insulator / Superconductor interface

  Fu and Kane, PRL **100**, 096409 (2008)
  Akhmerov *et al.*, PRL **102**, 216404 (2009)

- Probing helical edges states by Cooper pairs injection

  P. Adroguer *et al.*, PRB82, 081303 (2010)



- Topological Superconductivity /Superfluidity

  Wray et al., (2008)
  Hor et al., PRL **104**, 057001 (2010)

Thank You for your attention !