RWTH AACHEN
RHEINISCH-WESTFÄLISCHE TECHNISCHE HOCHSCHULE AACHEN

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DFG-FG 912

Topological properties in solids probed by Experiment

- Quantum Hall effect
- 2D TIs
- Weak Topological Insulators
- Strong topological insulators
- …

JARA | FIT
Fundamentals of Future Information Technology

Vienna, 04.08.2014

What is Topology ?

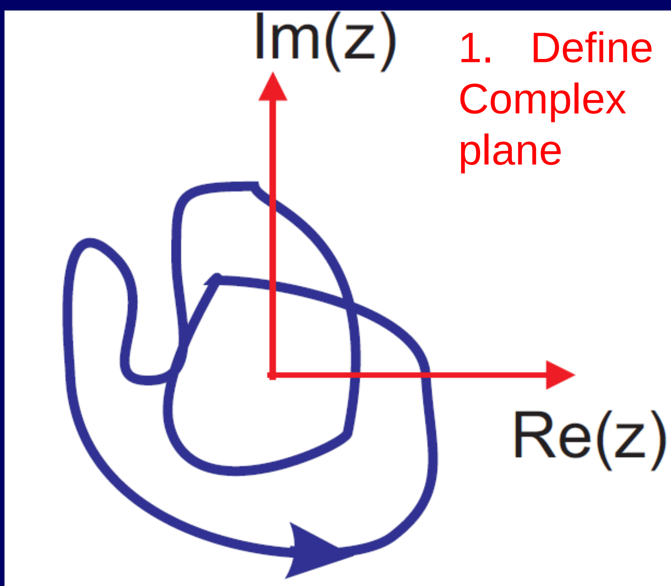
Wikipedia: Topology is the study of continuity and connectivity

… homeomorphism ….
fiber bundles …
….. Pontryagin classes
Haussdorf dimension
… Massey product

What is Topology ?

Idea: distinguish geometrical objects by integer numbers

Example:
Winding number of closed path



1. Define Complex plane

How often does the path wind around P, which is never touched ?

2. Path coordinate $t \in [0,1)$

$$z(t) = |z(t)| \cdot e^{i\phi(t)}$$

3. Find topological Invariant

$$Q(z) = \frac{1}{2\pi i} \int_0^1 \frac{dz(t)/dt}{z(t)} dt$$

4. Proof correctness

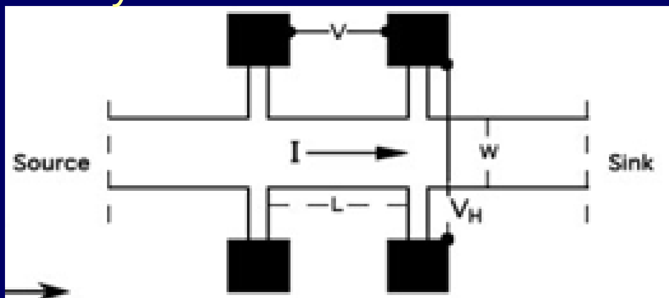
$$Q(z) = \frac{1}{2\pi i} \int_0^1 \frac{d}{dt} \log(z(t)) dt$$

$$= \frac{1}{2\pi i} [\log(z(t))]_0^1 = \frac{1}{2\pi i} \log\left(\frac{|z(1)|e^{i\phi(1)}}{|z(0)|e^{i\phi(0)}}\right)$$

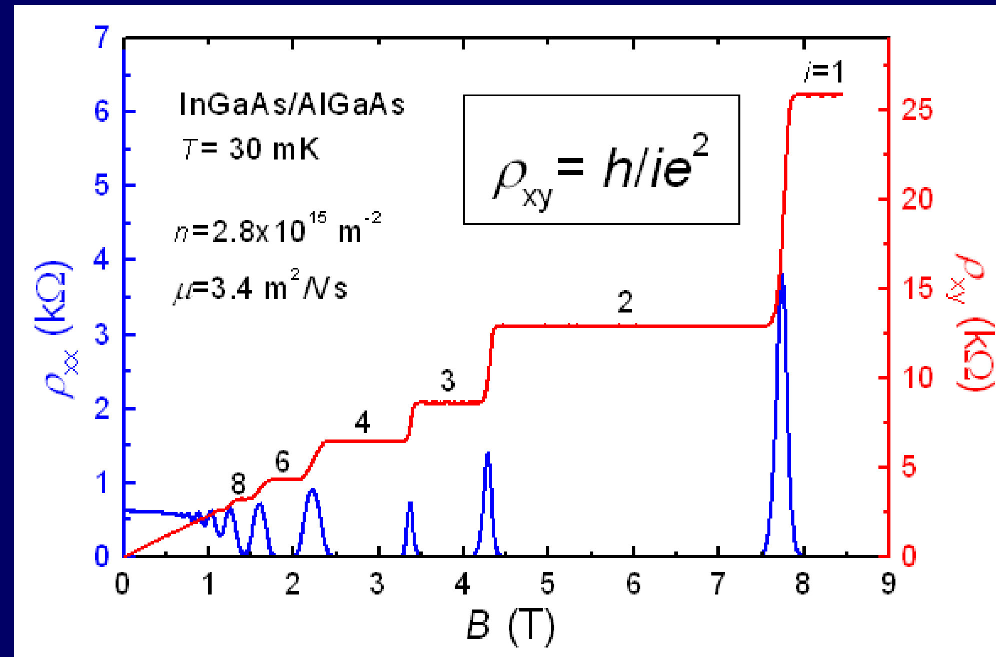
$$= \frac{1}{2\pi i} \cdot (\log(e^{i\phi(1)}) - \log(e^{i\phi(0)})) = \frac{\phi(1) - \phi(0)}{2\pi}$$

Topology in Solids: quantum Hall effect

2D system



v. Klitzing et al., PRL 45, 494 (80), …



- accurate mesurement of h/e^2 (precision: 10^{-10})

Thouless et al., PRL 49, 405 (82)

$$
\begin{aligned}
j_y &= -e \iint_{MBZ} \frac{dk_x dk_y}{(2\pi)^2} \sum_\alpha v_y^\alpha \\
&= \frac{E_x e^2}{h} \underbrace{\iint_{MBZ} \frac{dk_x dk_y}{(2\pi)i} \sum_\alpha \left(\langle \frac{\partial u^\alpha}{\partial k_y} | \frac{\partial u^\alpha}{\partial k_x} \rangle - \langle \frac{\partial u^\alpha}{\partial k_x} | \frac{\partial u^\alpha}{\partial k_y} \rangle \right)}_{\text{Chern number } n}
\end{aligned}
$$

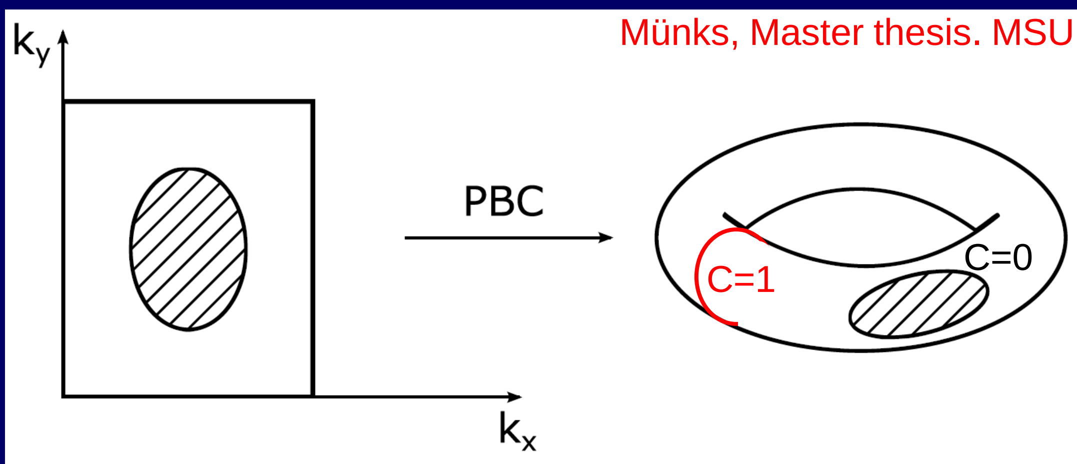
Chern number is a distinct integer,
if the system is gapped,
i.e. a band is either completely occupied or completely empty

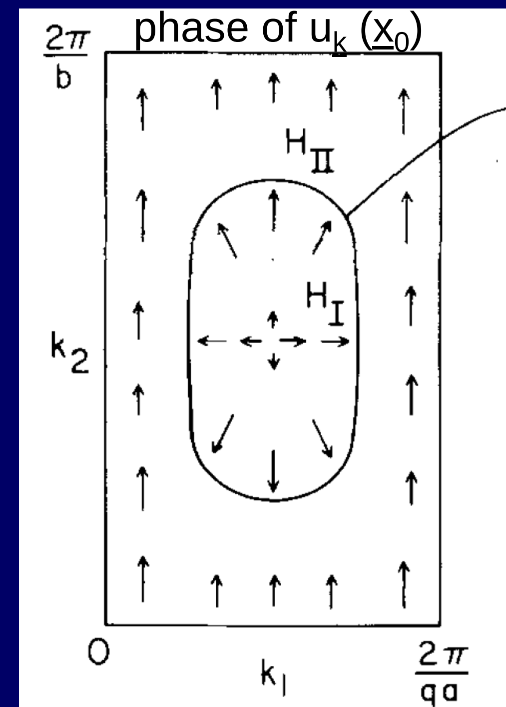
Chern number = integer: the argument

1) Define magnetic Brilloun zone (MBZ) by integer number of flux quanta inside each unit cell

$\Rightarrow$ wave function has zeros inside the unit cell (Aharonov Bohm phase $\neq 0$)

2) Combination with required periodicity of MBZ requires a <u>phase mismatch</u> around the zero for a particular real space <u>x</u>





Kohmoto, Ann. Phys. 160, 343 (85)

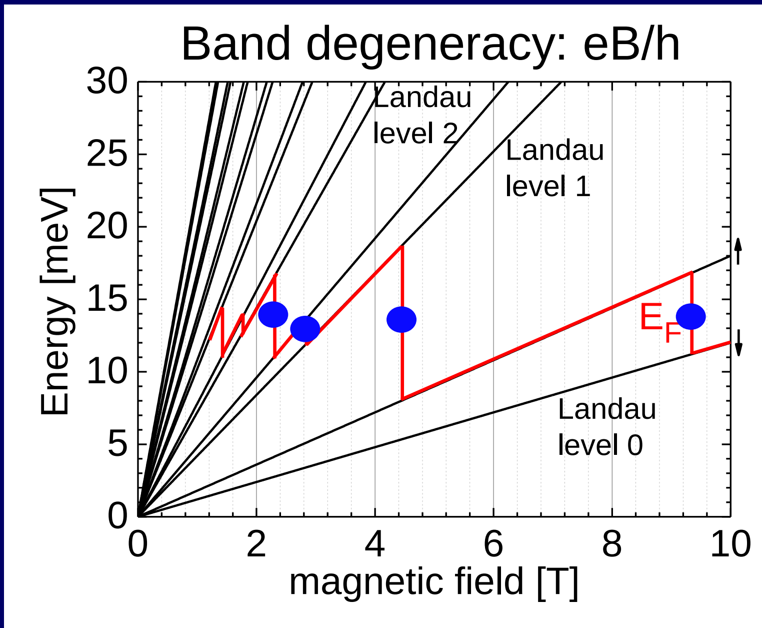
3) Integral of the <u>**gradient of the phase mismatch**</u> along the interface has to be single valued: 0, 2π, 4π …

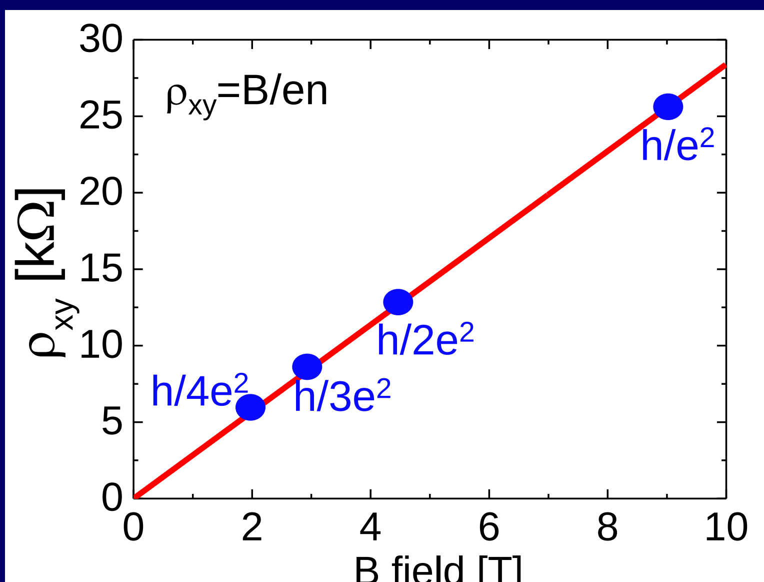
4) By Stokes theorem, this is identical to the Chern number

$$\underbrace{\iint_{MBZ} \frac{dk_x dk_y}{(2\pi)i} \sum_\alpha \left(\langle \frac{\partial u^\alpha}{\partial k_y} | \frac{\partial u^\alpha}{\partial k_x} \rangle - \langle \frac{\partial u^\alpha}{\partial k_x} | \frac{\partial u^\alpha}{\partial k_y} \rangle \right)}_{\text{Chern number } n}$$

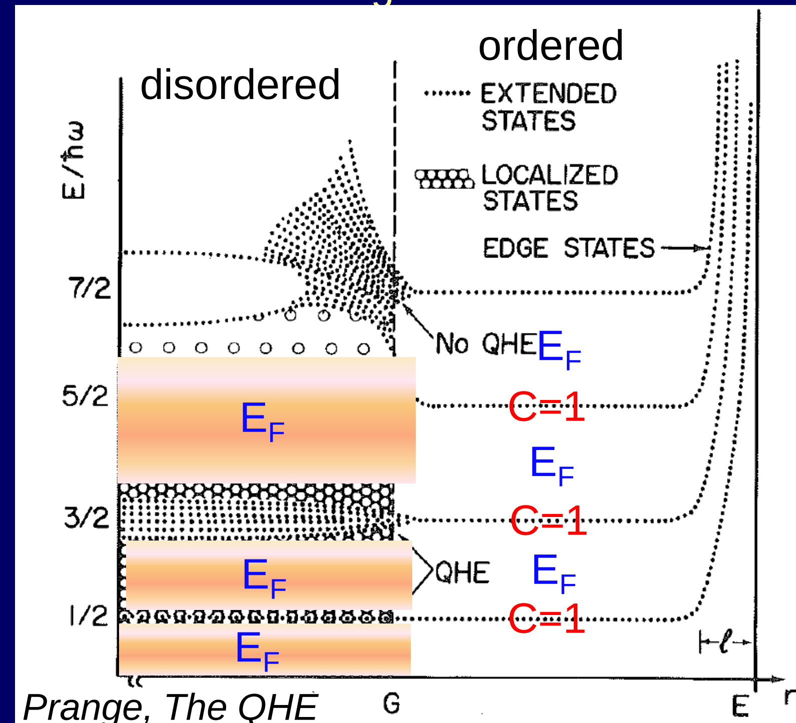
Requirement: the band must be full, such that the MBZ is densely occupied

Chern number = integer: filling the band





adding disorder



$$\sigma_{xy} = \frac{ie^2}{\hbar}\left[\left\langle \frac{\partial\phi_0}{\partial\theta}\middle|\frac{\partial\phi_0}{\partial\varphi}\right\rangle - \left[\left\langle \frac{\partial\phi_0}{\partial\varphi}\middle|\frac{\partial\phi_0}{\partial\theta}\right\rangle\right]\right]$$

Ground state Wave function

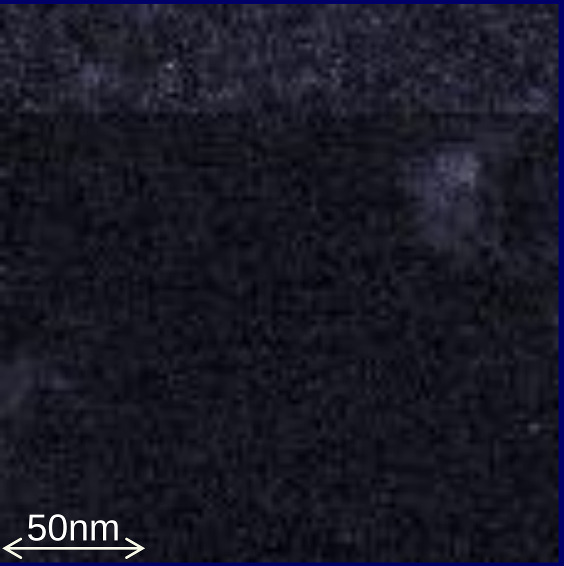
boundary phase factors

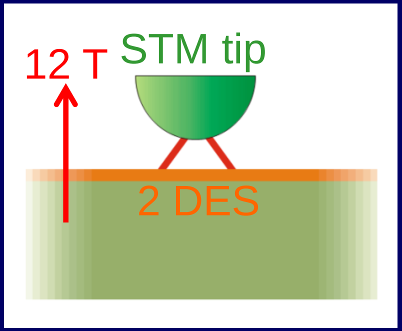
Conductance with E_F at localized states does not depend on boundary conditions ⇒

$$\bar{\sigma}_{xy} = \frac{e^2}{h}\int_0^{2\pi}\int_0^{2\pi} d\theta\, d\varphi \frac{1}{2\pi i}\left[\left\langle \frac{\partial\phi_0}{\partial\varphi}\middle|\frac{\partial\phi_0}{\partial\theta}\right\rangle - \left\langle \frac{\partial\phi_0}{\partial\theta}\middle|\frac{\partial\phi_0}{\partial\varphi}\right\rangle\right]$$

Quantum Hall winding number in real space

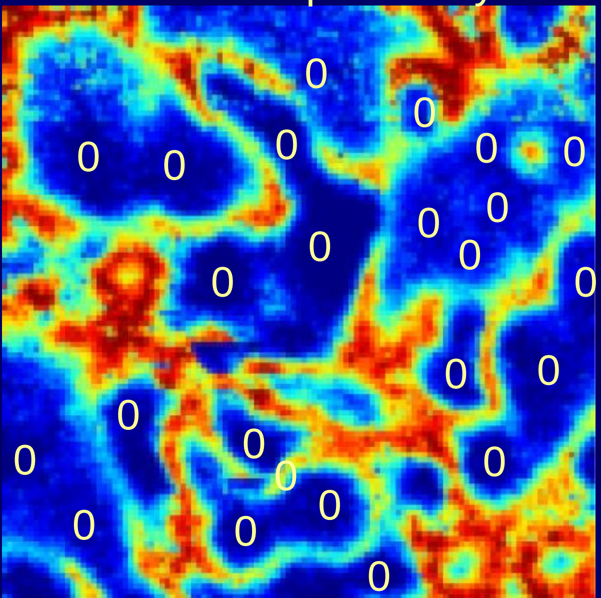
2D LDOS at B= 12 T, 0.3 K





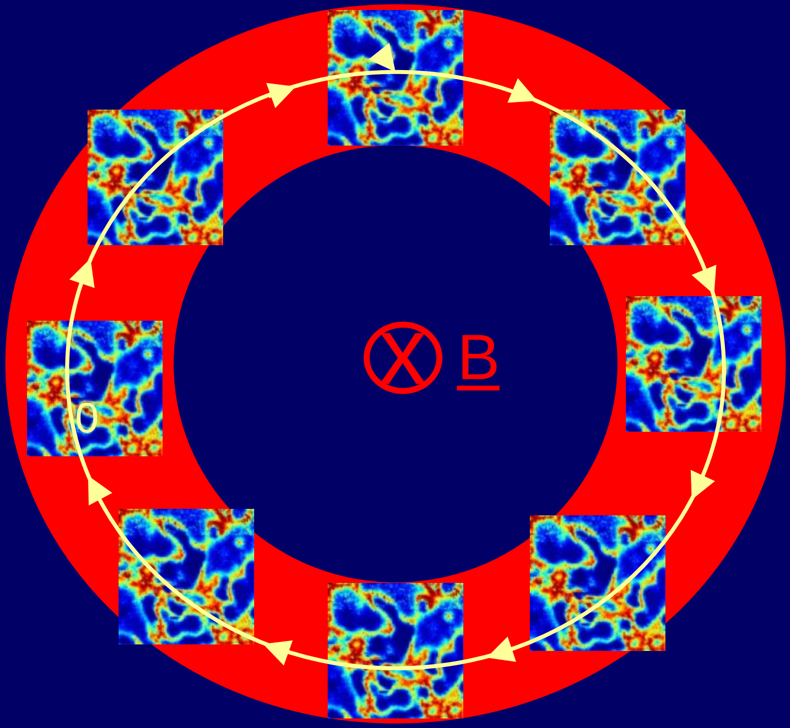
PRL 101, 256802 (08)

Extended state probed by STM (C=1)



One node (0)
per flux quantum
in extended state

Corbino-Geometry

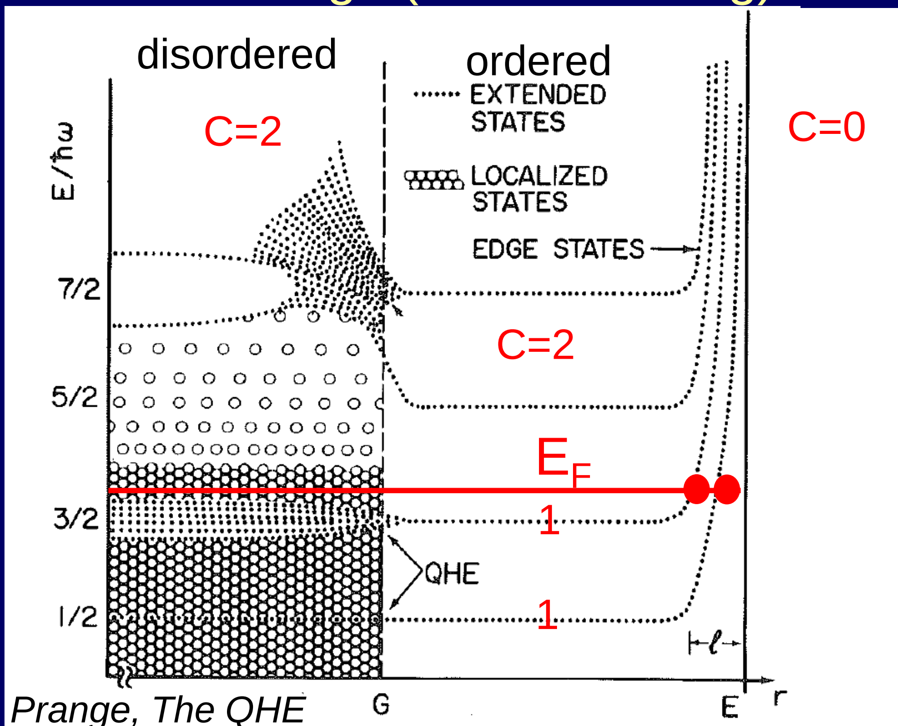


Prediction: one more flux quantum =
one node encircles the flux =
winding number of zeros

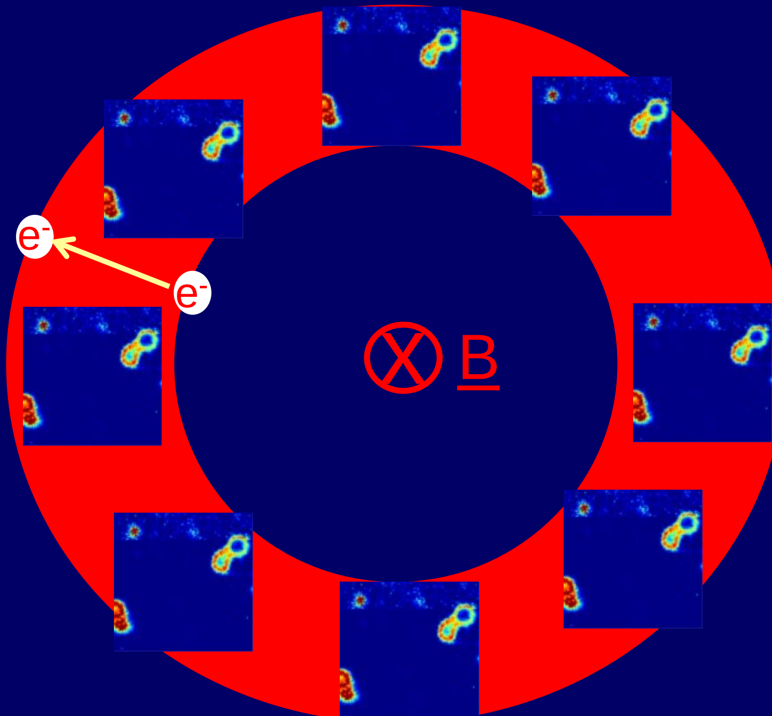
Arovas et al. PRL 60, 619 (85)

Bulk edge corespondance

Where is the charge of the quantized Hall voltage (bulk insulating) ?



Corbino (insulating)



Answer: at the topological phase boundary, where different Chern numbers clash

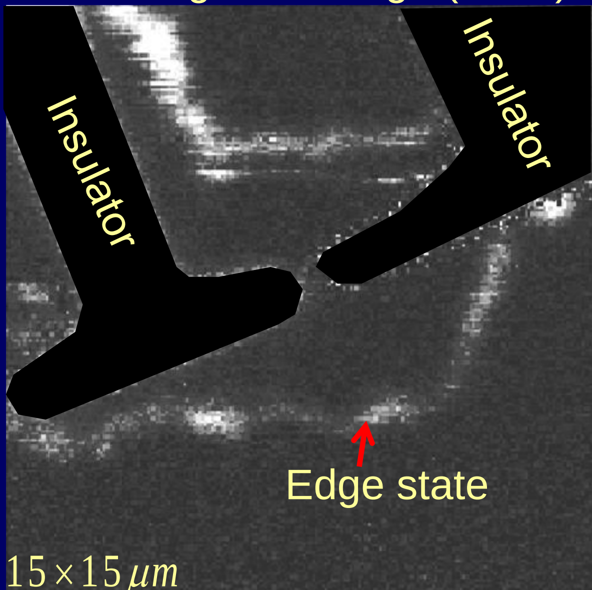
Laughlins argument: one more flux moves charge from inner to outer rim without energy cost (WF identical)

$\Rightarrow$ ….$\Rightarrow$ one chiral edge state per Chern number

Seeing the edge state

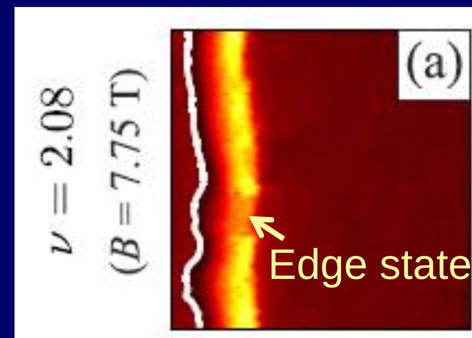
Edge state = „metallic“ area of high compressibility

Scanning SET image (2.2 T)

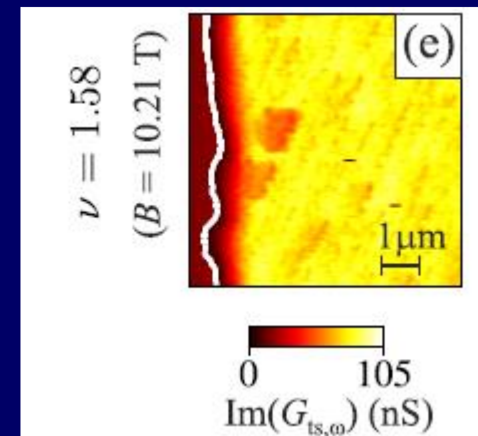


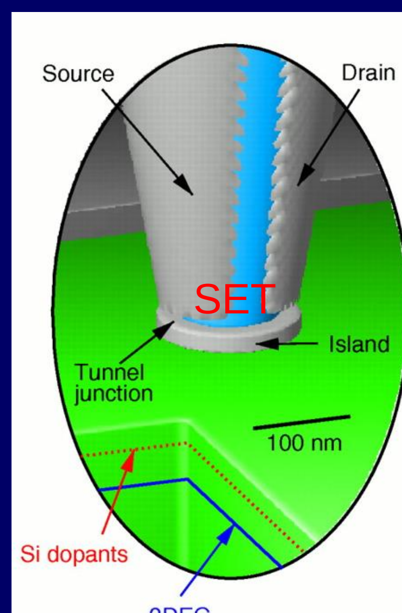
courtesy A. Yacoby (Harvard)

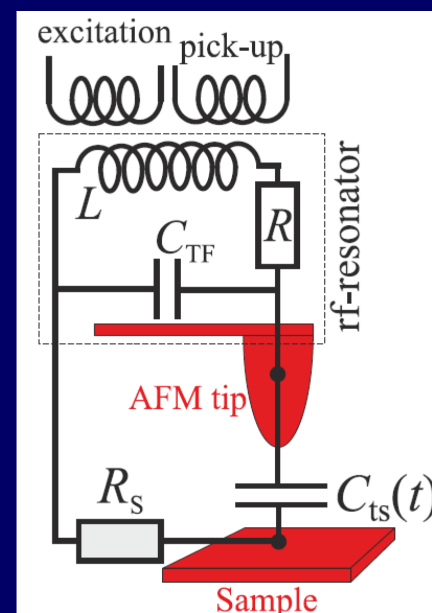
Scanning capacitance image



Suddards et al.
NJP 14, 083015 (12)







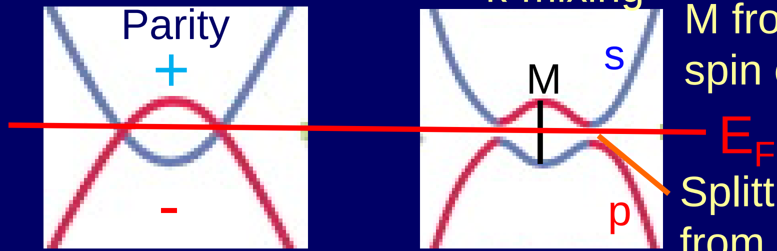
- Local potential changes SET conductance
- Metallic edge state screens backgate potential for SET

Part II
2D Topological Insulators
(B = 0 T)

Topology in 2D at B = 0 T

Make a band gap in 2D by mixing two bands
with different parity

Inverted bands + k-mixing



M from spin orbit

Splitting from k·p

k-space

Formally:

Spin 1

$$\mathcal{H} = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}$$

Spin 2

Bernevig et al, Science 314, 1757 (05)

$$h(k) = \epsilon(k)\mathrm{I}_{2\times 2} + d_a(k)\sigma^a$$

Pauli matrix for s,p

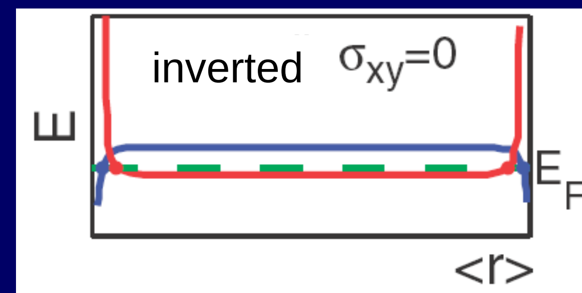
$$d_a(k) = (Ak_x, -Ak_y, M(k))$$
$$M(k) = M - B(k_x^2 + k_y^2),$$

Nodal line in k-space

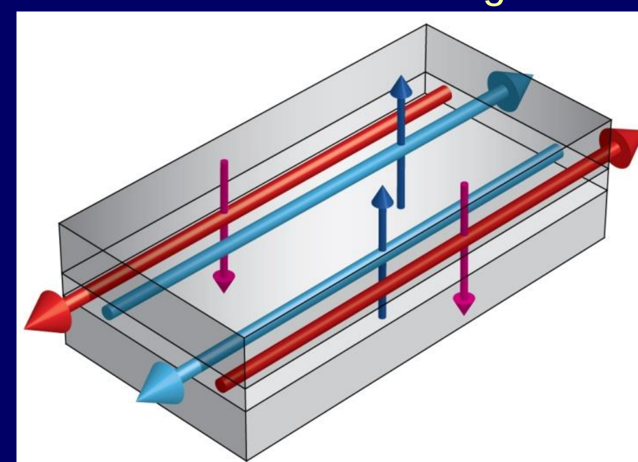
topological number for one „spin“

$$\sigma_{xy} = -\frac{1}{8\pi^2}\iint dk_x dk_y \hat{\mathbf{d}} \cdot \partial_{\mathbf{x}}\hat{\mathbf{d}} \times \partial_{\mathbf{y}}\hat{\mathbf{d}} \cdot e^2/h$$

$\Delta\sigma_{xy}$= +/- 1 for 0 < M < 4B (+: Spin 1, - Spin2)

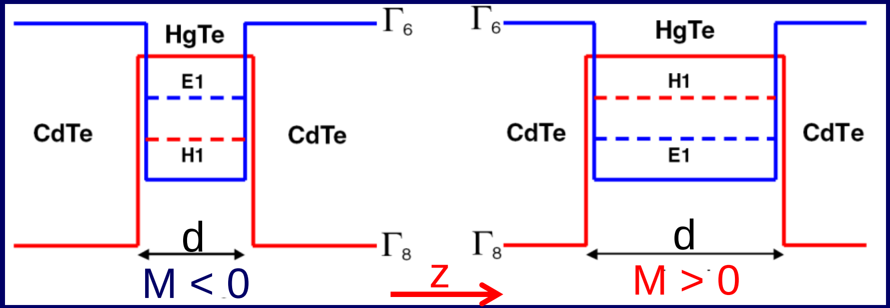


no backscattering



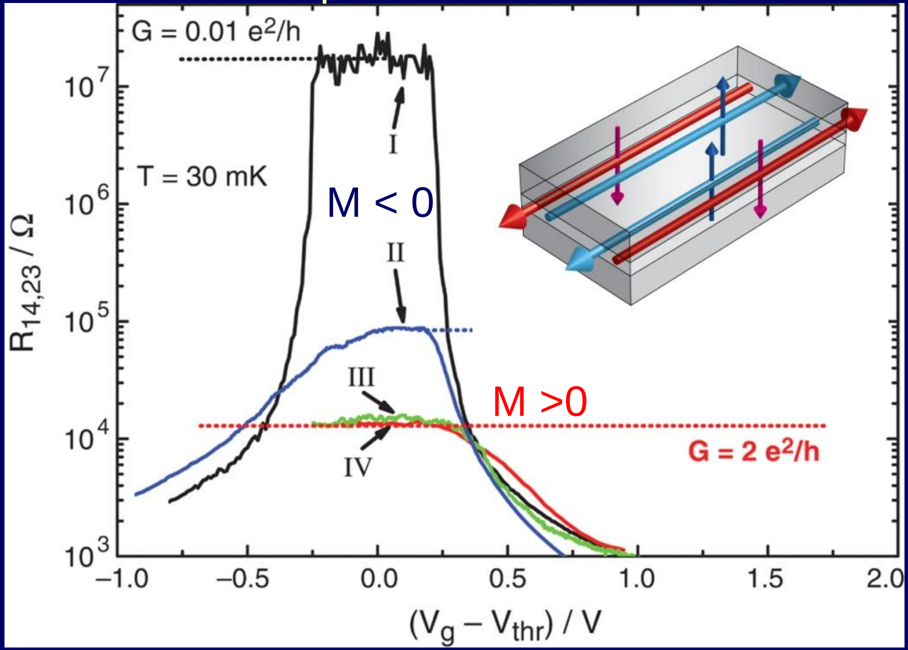
Experiment: non-trivial topology at B = 0 T

Tuning sign of M by z-confinement



1st transport: Ong et al. PRB 28, 2289(83)

4-point resistance

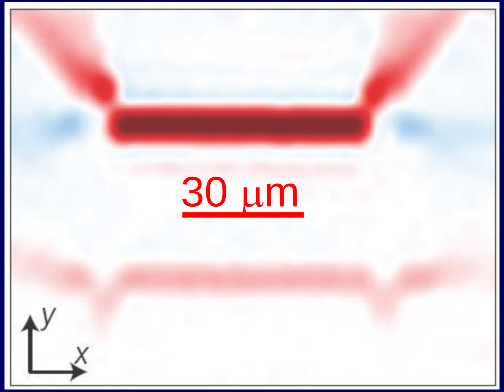


König et al., Science 318, 767 (07)

$$\lambda_{1,2}^2 = k_x^2 + F \pm \sqrt{F^2 - (M^2 - E^2)/B_+B_-},$$
$$F = \frac{A^2 - 2(MB + ED)}{2B_+B_-}.$$

Scanning SQUID (3 K)

within gap

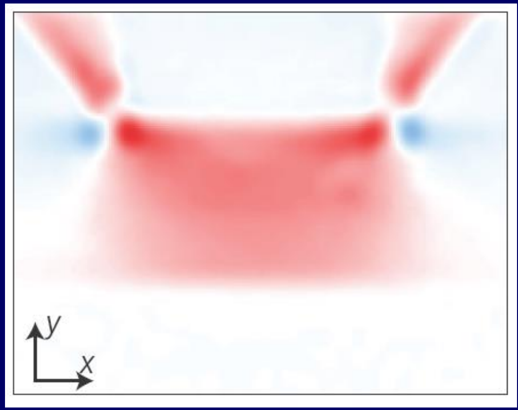


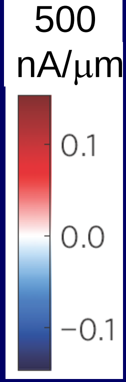
calculated width of edge state: 200 nm

Zhou et al., PRL 101, 246807 (08)

M > 0

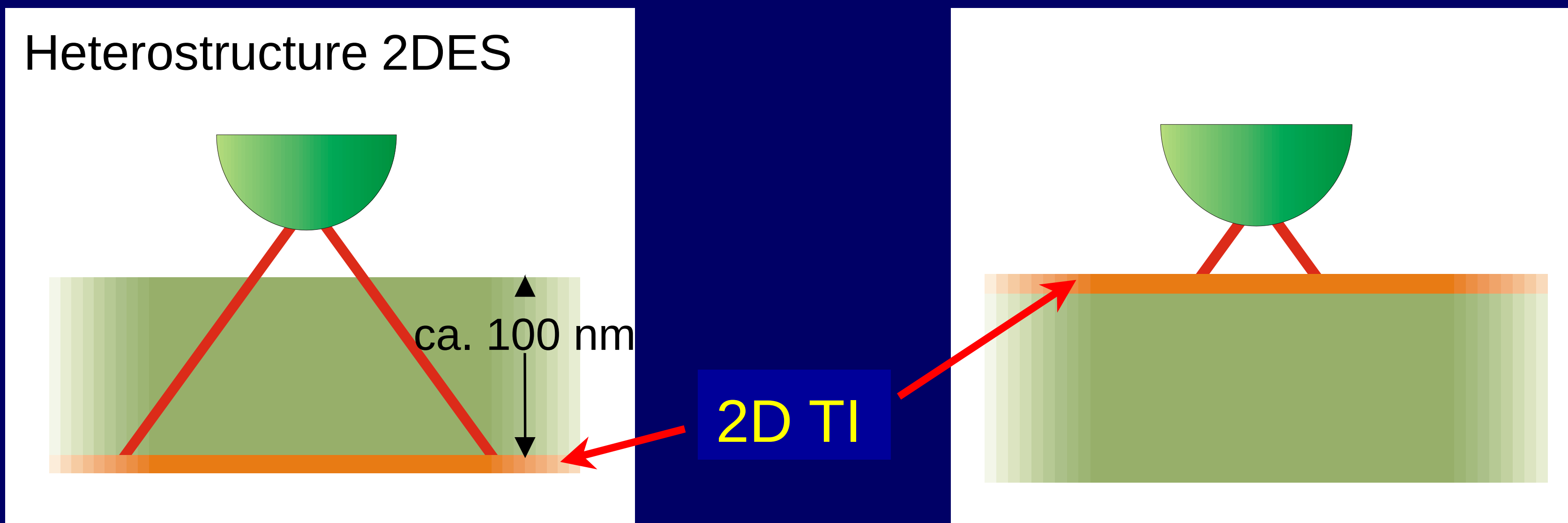
within bulk con-duc-tion band





Nowack et al., Nature Mat. 12, 787 (13)

Scanning tunneling spectroscopy ?
(LDOS with high resolution)

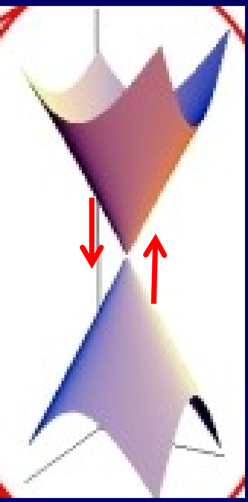


tunneling current: 10^{-50} A
STS-Resolution: 100 nm

tunneling current: 10^{-10} A
STS-Resolution < 0.1 nm

Stacked 2D topological insulators = weak 3D topological insulators

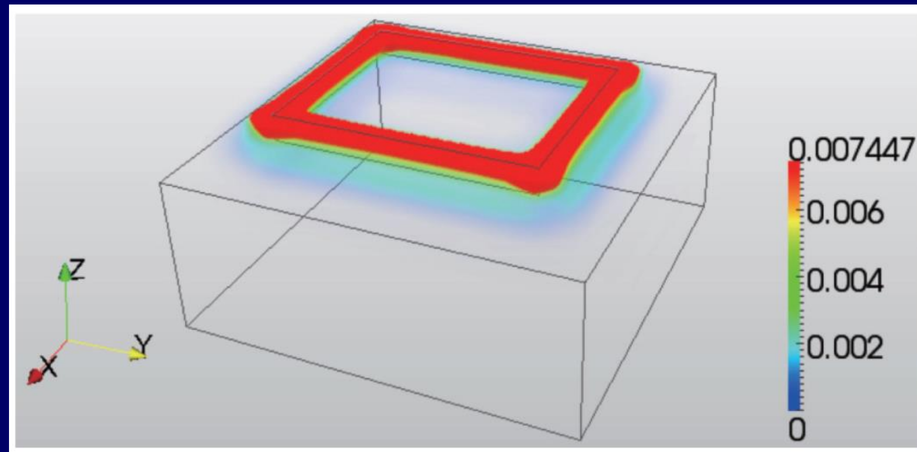
Graphene
Dirac cone



Invert by
Spin-orbit

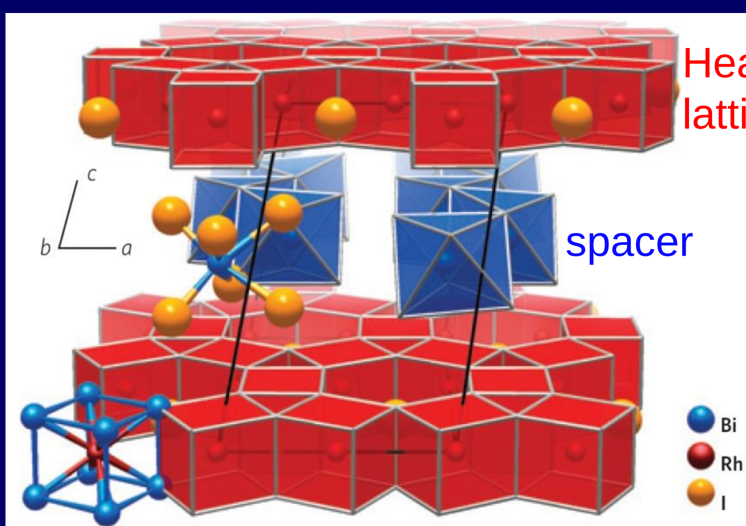
Gap by
confinement
(interlayer
interaction)

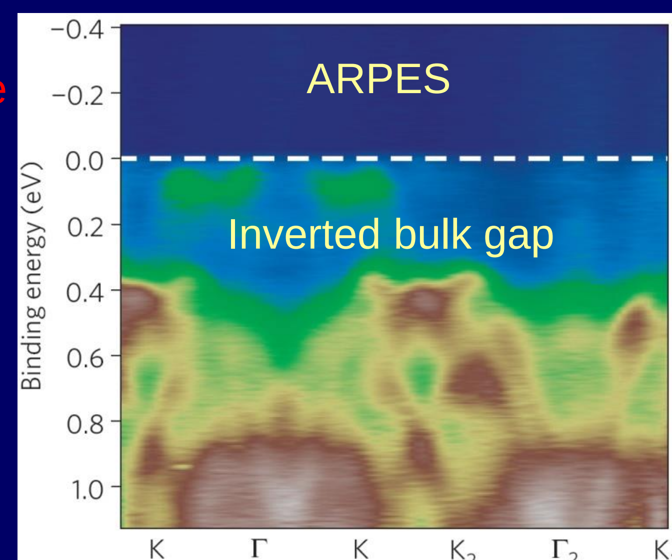
Kane et al.,
PRL 95,
226801 (05)



Yoshimura et al., PRB 88, 045408 (13)

First experimental weak TI: $Bi_{14}Rh_3I_9$ cleaved at the dark side

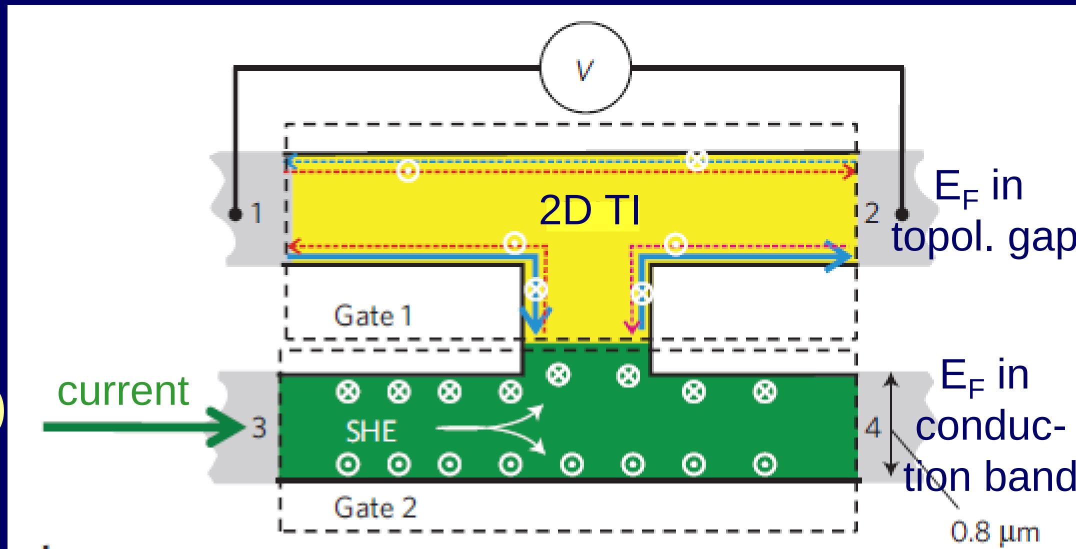


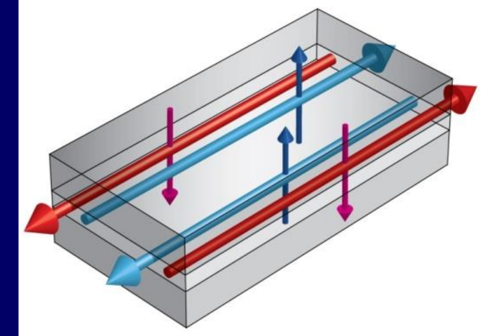


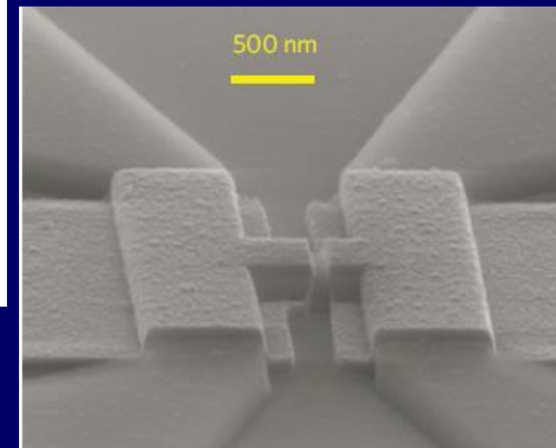
Rasche et al., Nature Mat. 12, 422 (13)

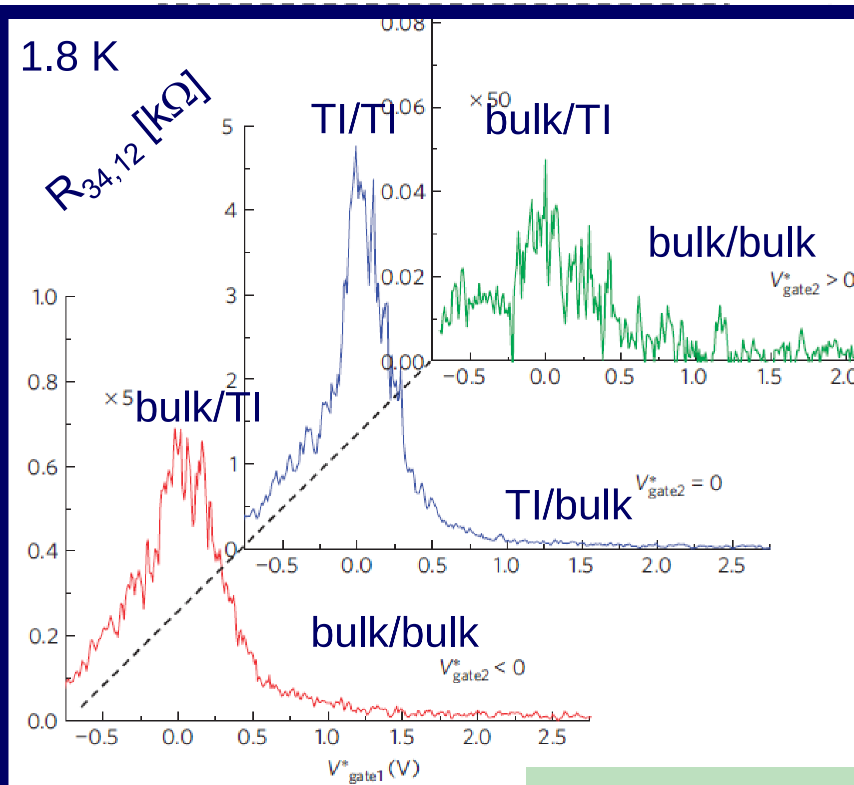
Probing spin transport in 2D TI

Non local
voltage
meas.
(2D HgTe)







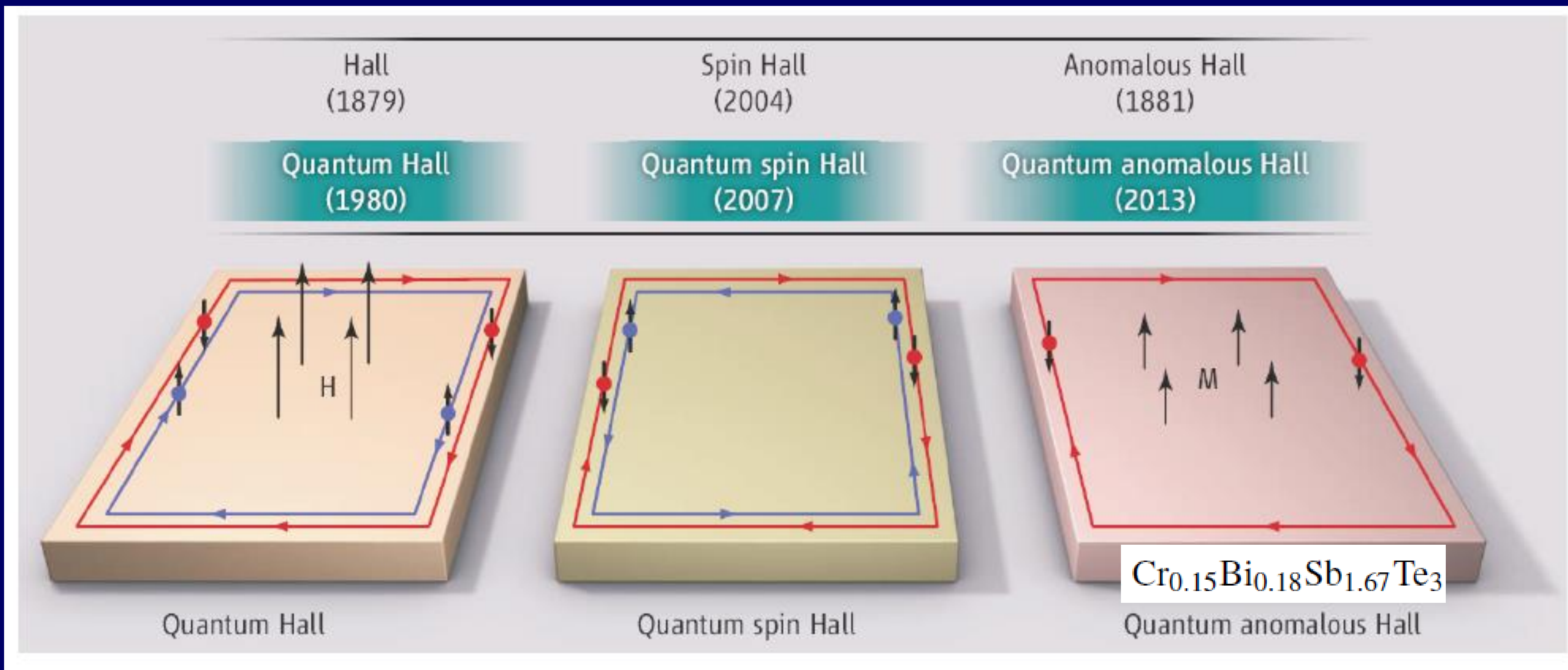


Strong signal if both areas TI

small signal,
if one area =TI
one area = bulk

Brüne et al.,
Nature Mat.
8, 485 (12)

Quantum anomolous Hall effect



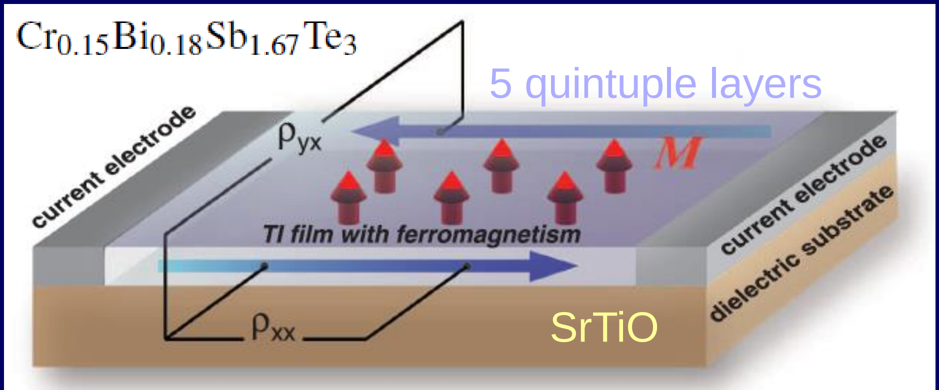
$$H_\uparrow(\underline{k}) = H_\downarrow^*(-\underline{k})$$

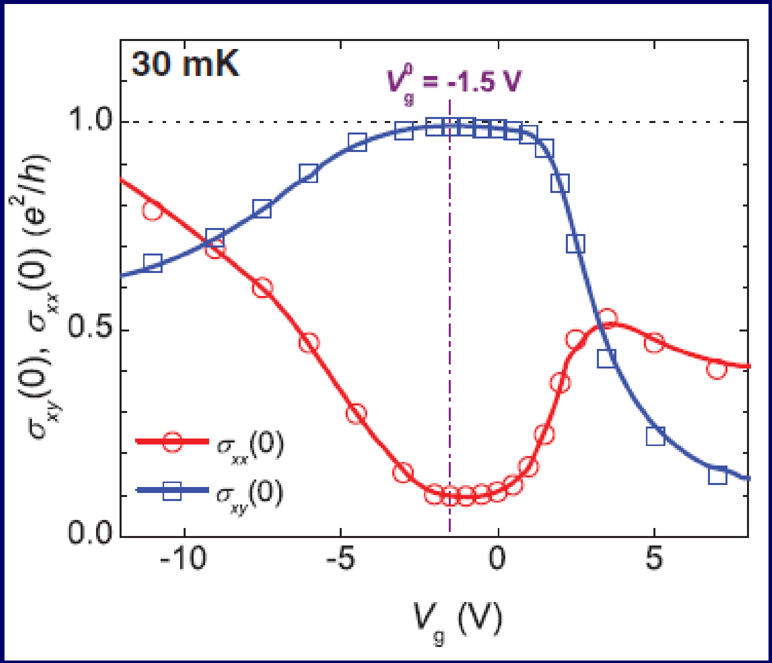
$$H_\uparrow(\underline{k}) \neq H_\downarrow^*(-\underline{k})$$

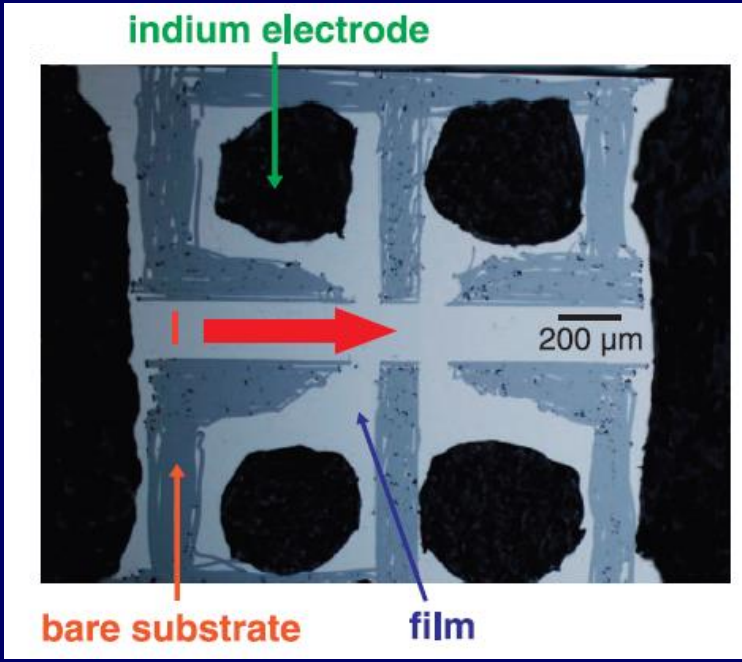
$$\mathcal{H} = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}$$

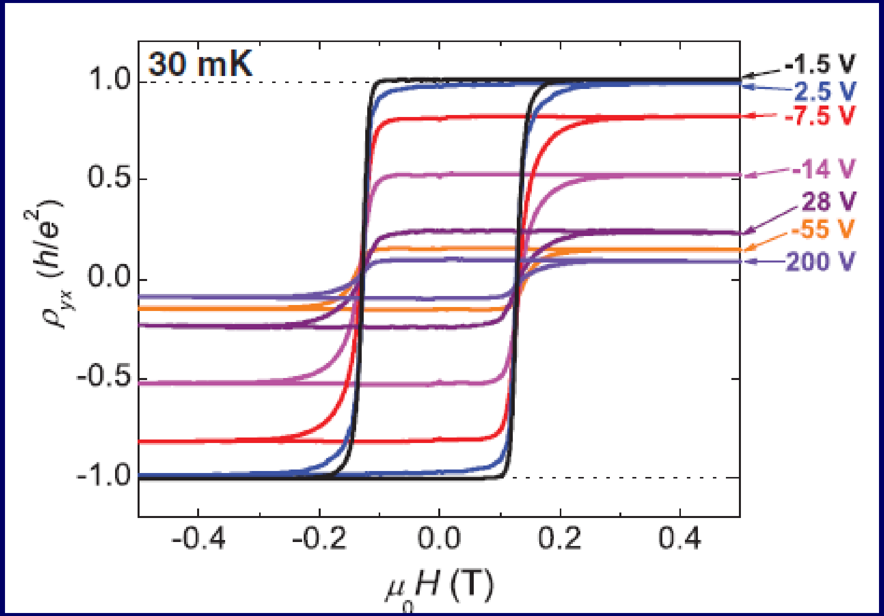
Quantum anomolous Hall effect (Exp.)

A ferromagnetic 2D TI









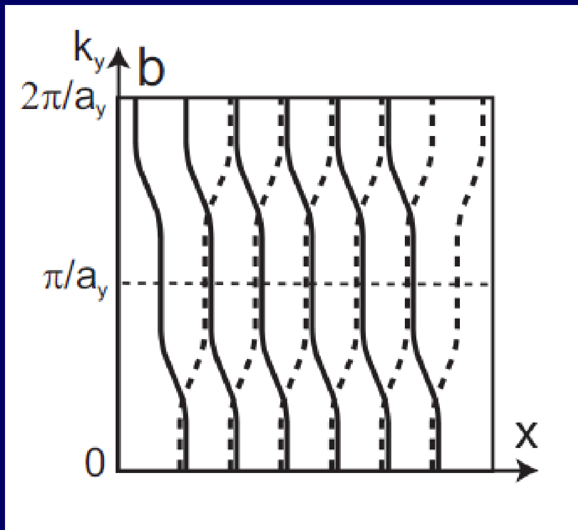
Chang et al., Science 340, 167 (13)

Part III
3D Topological Insulators
(B = 0 T)

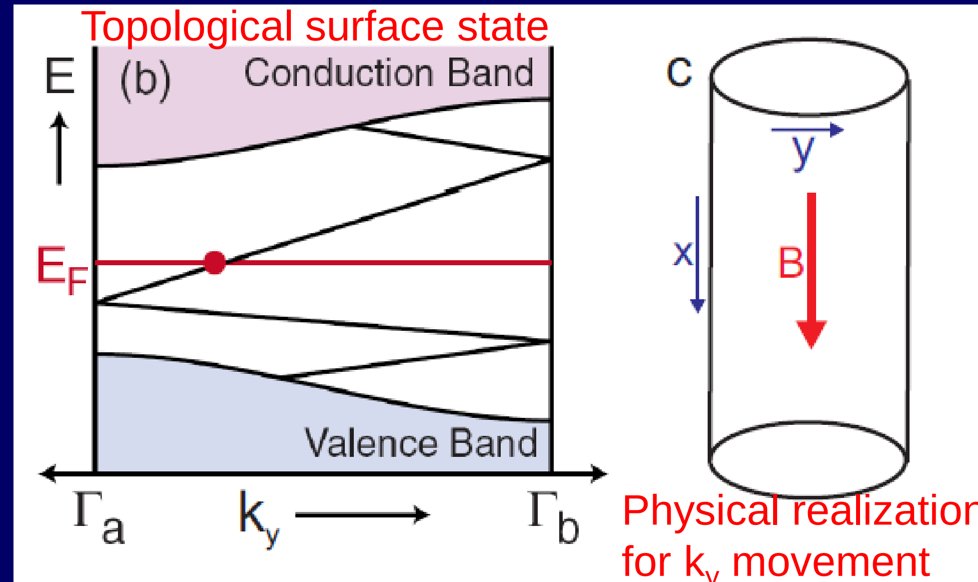
Fu Kane Mele
PRL 98, 106803 (07)
PRB 74, 195312 (07)

2D/3D Topological Insulators

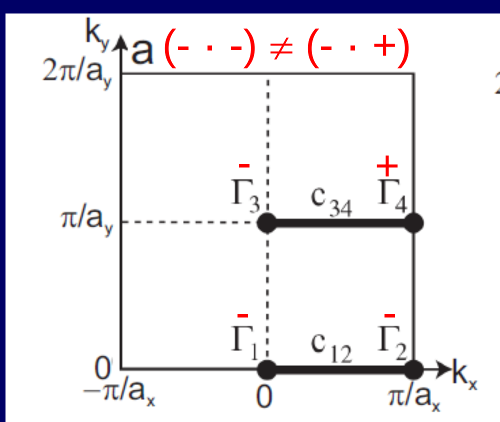
Kramers pair movement in 2D ribbon



Spin moved from left to right
with band gap in bulk =
spin pol. edge state required at E_F

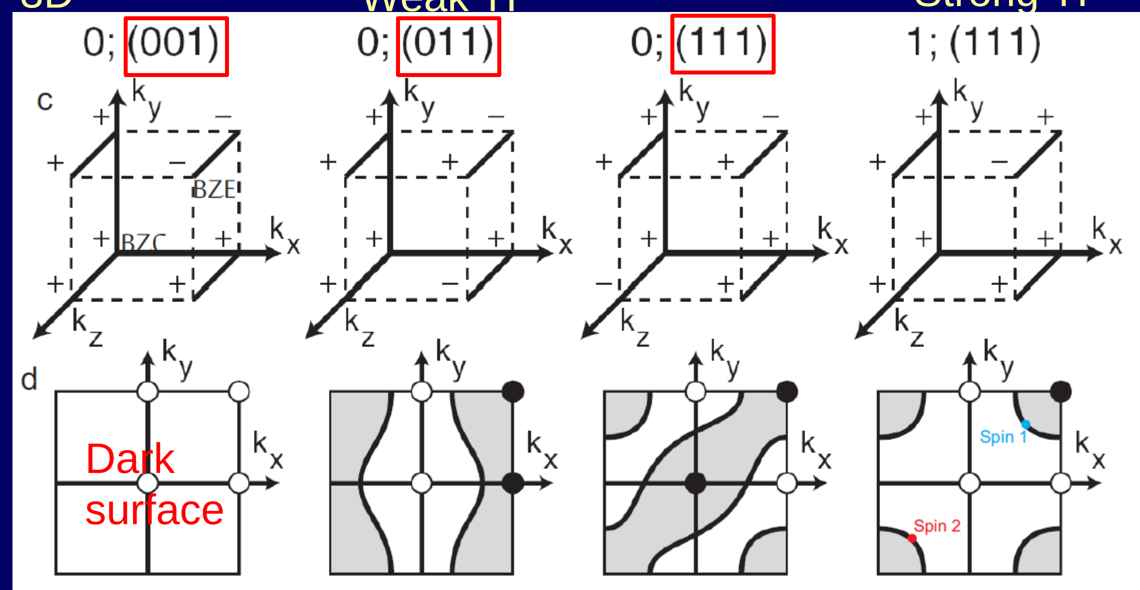


Edge state = bulk band property



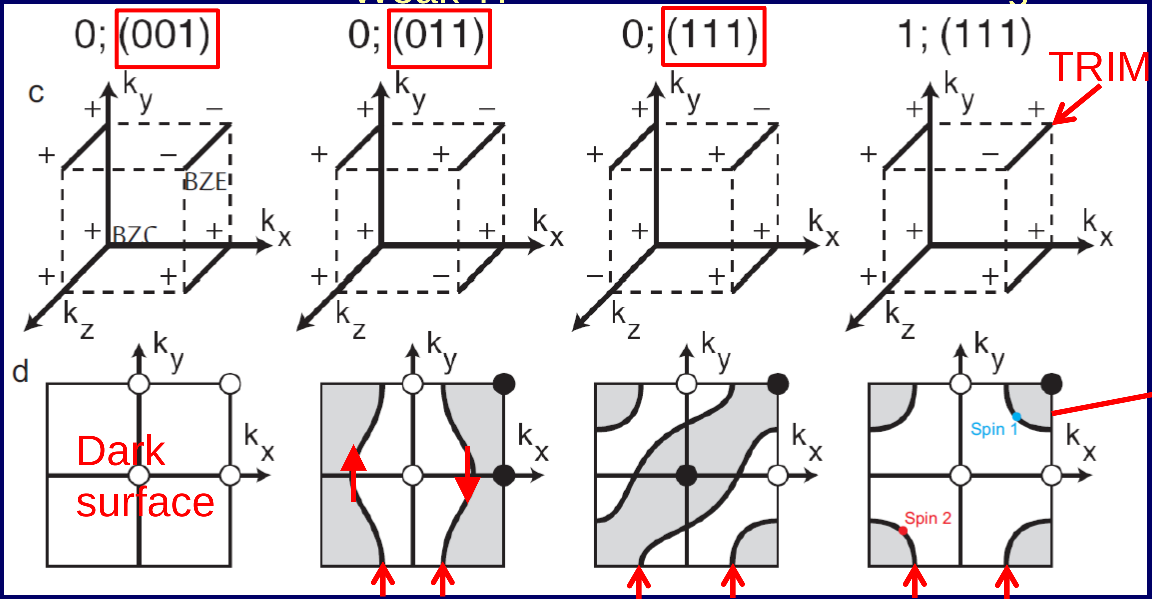
States important for movement
(Pfaffian vs. Determinant at TRIM)

3D Weak TI Strong TI



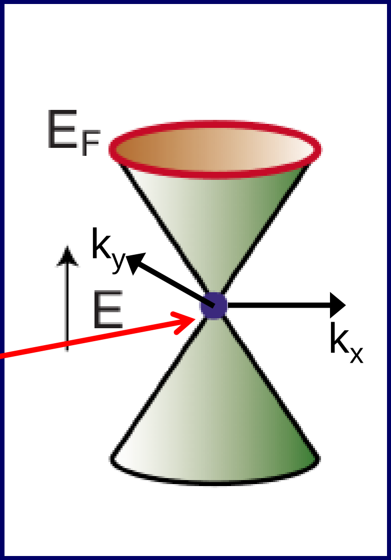
3D Topological Insulators

3D Weak TI Strong TI

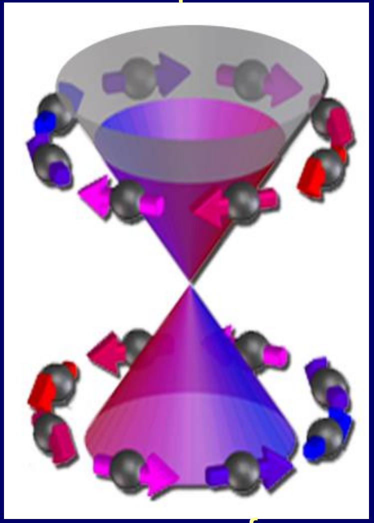


required surface states at E_F, all spin polarized
and time reversal invariant

E(k) dispersion



+ spin



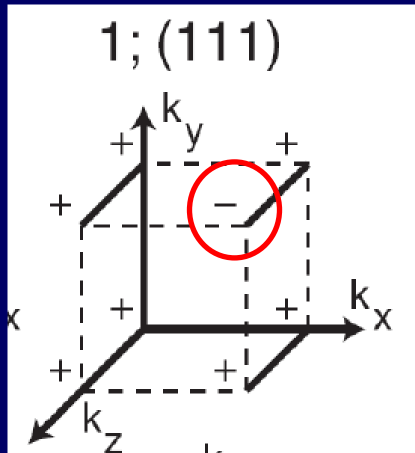
upper surface

only relative Bloch wave function phases
at TRIMs matter

Bulk inversion symmetry of crystal $\Rightarrow$
Sign at TRIM = product of
parities of all states below the gap

TRIM = Time reversal invariant momenta ($\underline{k}$ = -$\underline{k}$)

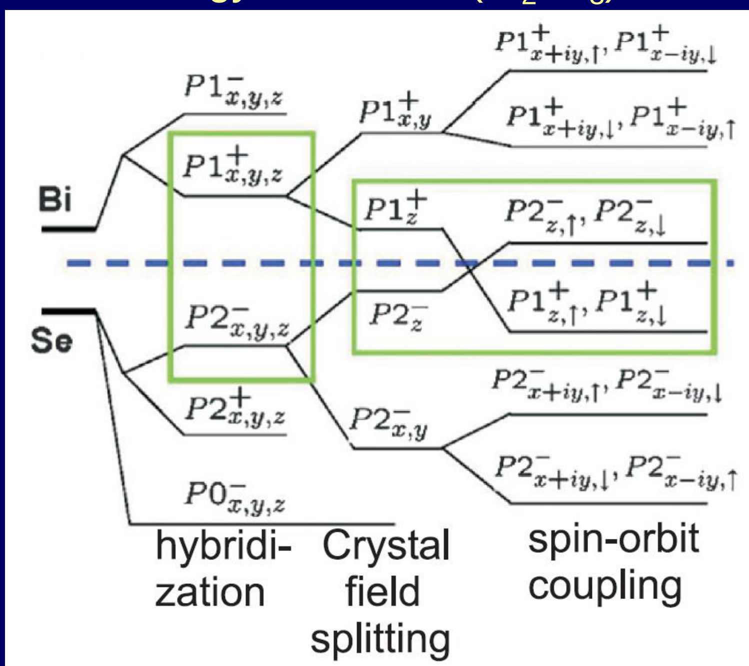
Materials: 3D Topological Insulators



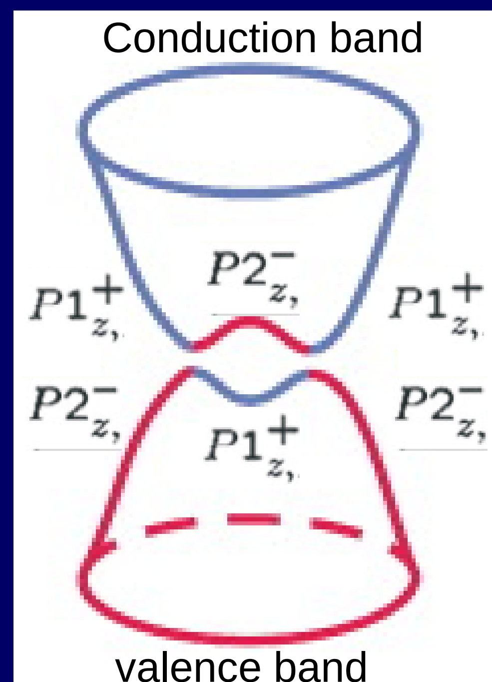
Bulk inversion symmetry of crystal ⇒
Sign at TRIM = product of
parities of all states below the gap

⇒ Band inversion (= exchanged parity)
at 1 TRIM (typically Γ)

Energy levels at Γ (Bi_2Se_3)



Li et al., Rev. Mod. Phys 83, 1057 (11)

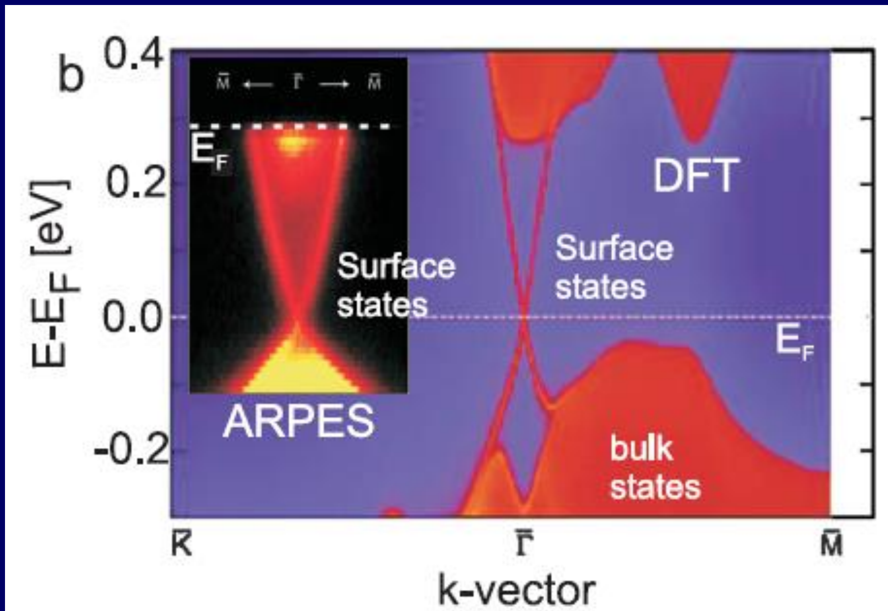


Good means to
invert bands

Spin-orbit interaction
electron-electron
interaction
…

Exp. proof: 3D Topological Insulators

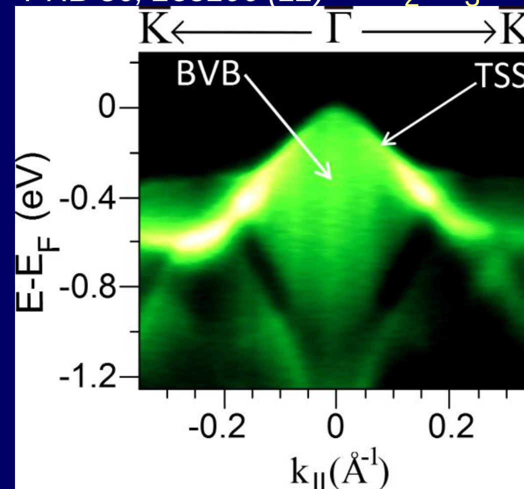
Zhang et al., Nature Phys. 5, 438 (09)

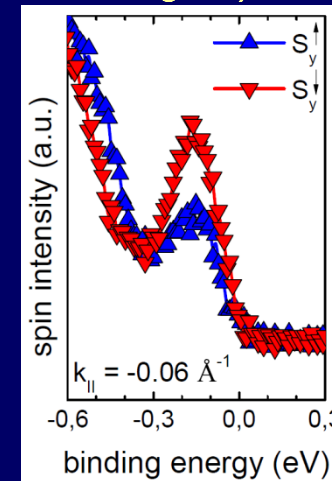


Our contribution

PRB 86, 235106 (12) Sb_2Te_3

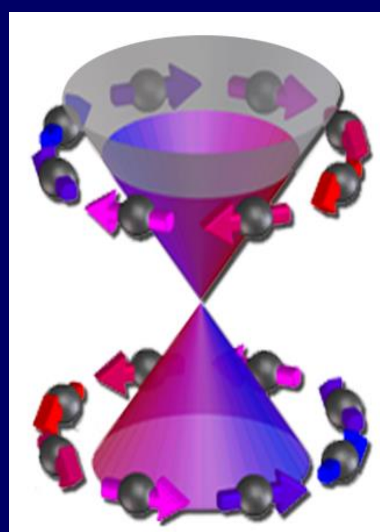
Spin polarization (disentangled): 85 %



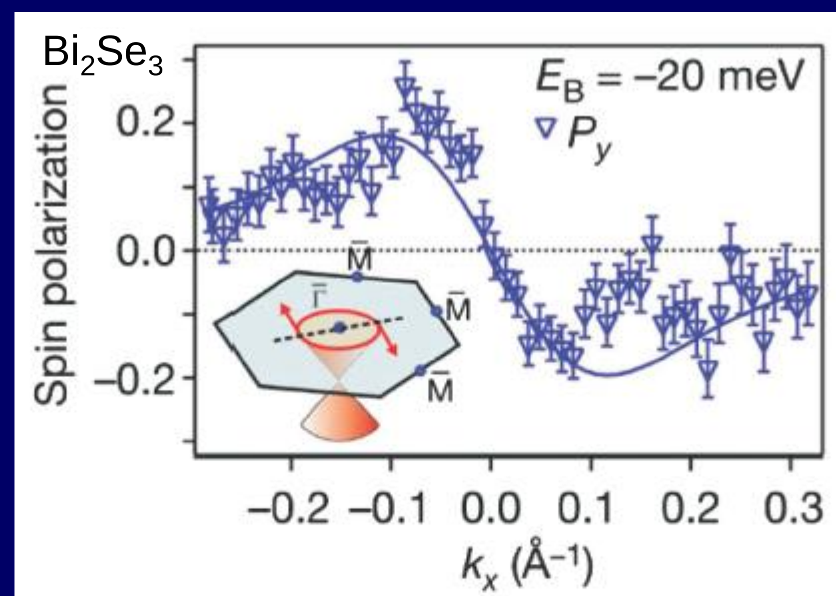


Science 325, 178 (09)

ARPES Bi_2Te_3



E (k) with spins



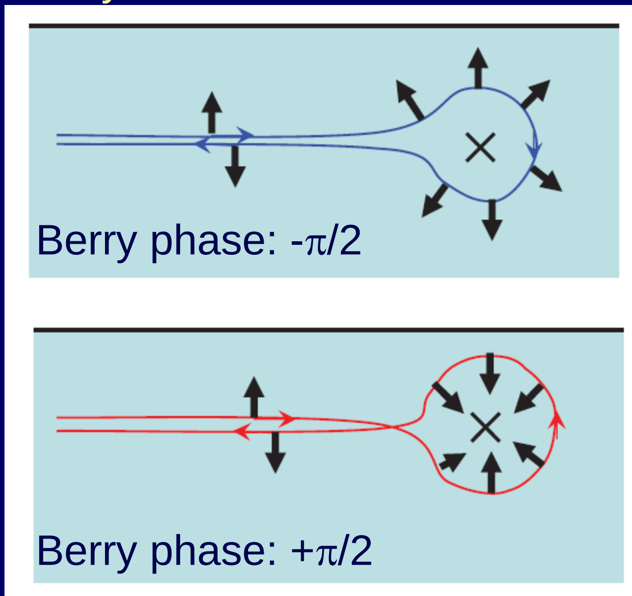
Materials: topological insulators

Type	Material	Band gap	Bulk transport	Remark	Reference
2D, $\nu = 1$	CdTe/HgTe/CdTe	< 10 meV	insulating	high mobility	26)
2D, $\nu = 1$	AlSb/InAs/GaSb/AlSb	~4 meV	weakly insulating	gap is too small	64)
3D (1;111)	$Bi_{1-x}Sb_x$	< 30 meV	weakly insulating	complex S.S.	31,35)
3D (1;111)	Sb	semimetal	metallic	complex S.S.	34)
3D (1;000)	Bi_2Se_3	0.3 eV	metallic	simple S.S.	79)
3D (1;000)	Bi_2Te_3	0.17 eV	metallic	distorted S.S.	80,81)
3D (1;000)	Sb_2Te_3	0.3 eV	metallic	heavily p-type	82)
3D (1;000)	Bi_2Te_2Se	~0.2 eV	reasonably insulating	ρ_{xx} up to 6 Ωcm	96,99,101)
3D (1;000)	$(Bi,Sb)_2Te_3$	< 0.2 eV	moderately insulating	mostly thin films	168)
3D (1;000)	$Bi_{2-x}Sb_xTe_{3-y}Se_y$	< 0.3 eV	reasonably insulating	Dirac-cone engineering	103,104,187)
3D (1;000)	$Bi_2Te_{1.6}S_{1.4}$	0.2 eV	metallic	n-type	185)
3D (1;000)	$Bi_{1.1}Sb_{0.9}Te_2S$	0.2 eV	moderately insulating	ρ_{xx} up to 0.1 Ωcm	185)
3D (1;000)	Sb_2Te_2Se	?	metallic	heavily p-type	96)
3D (1;000)	$Bi_2(Te,Se)_2(Se,S)$	0.3 eV	semi-metallic	natural Kawazulite	186)
3D (1;000)	$TlBiSe_2$	~0.35 eV	metallic	simple S.S., largest gap	87–89)
3D (1;000)	$TlBiTe_2$	~0.2 eV	metallic	distorted S.S.	89)
3D (1;000)	$TlBi(S,Se)_2$	< 0.35 eV	metallic	topological P.T.	93,94)
3D (1;000)	$PbBi_2Te_4$	~0.2 eV	metallic	S.S. nearly parabolic	106,109)
3D (1;000)	$PbSb_2Te_4$	?	metallic	p-type	106)
3D (1;000)	$GeBi_2Te_4$	0.18 eV	metallic	n-type	96–98)
3D (1;000)	$PbBi_4Te_7$	0.2	metallic	heavily n-type	110)
3D (1;000)	$GeBi_4Te_7$	?	?	no data published yet	111)
3D (1;000)	$(PbSe)_5(Bi_2Se_3)_6$	0.5 eV	metallic	natural heterostructure	114)
3D (1;000)	$(Bi_2)(Bi_2Se_{2.6}S_{0.4})$	semimetal	metallic	$(Bi_2)_n(Bi_2Se_3)_m$ series	112)
3D (1;000)	$(Bi_2)(Bi_2Te_3)_2$	?	?	no data published yet	111)
3D TCI	SnTe	0.3 eV (4.2 K)	metallic	Mirror TCI, $n_M = -2$	54)
3D TCI	$Pb_{1-x}Sn_xTe$	< 0.3 eV	metallic	Mirror TCI, $n_M = -2$	140)
3D TCI	$Pb_{0.77}Sn_{0.23}Se$	invert with T	metallic	Mirror TCI, $n_M = -2$	138)
3D (1;111)?	SmB_6	20 meV	insulating	possible Kondo TI	118–121)
3D (0;001)?	$Bi_{14}Rh_3I_9$	0.27 eV	metallic	possible weak 3D TI	123)
3D (1;000)?	RBiPt (R = Lu, Dy, Gd)	zero gap	metallic	evidence negative	130)
Weyl S.M.?	$Nd_2(Ir_{1-x}Rh_x)_2O_7$	zero gap	metallic	too preliminary	135)

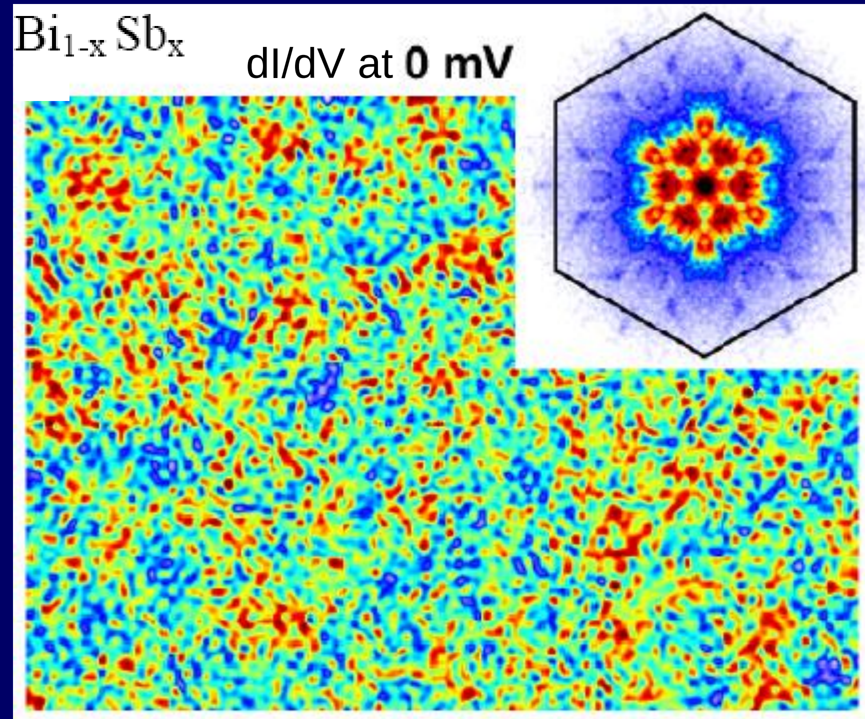
Y. Ando, J. Phys. Soc. Jap. 82, 102001 (13)

Detecting prohibited backscattering

Backscattering prohibited by destructive interference



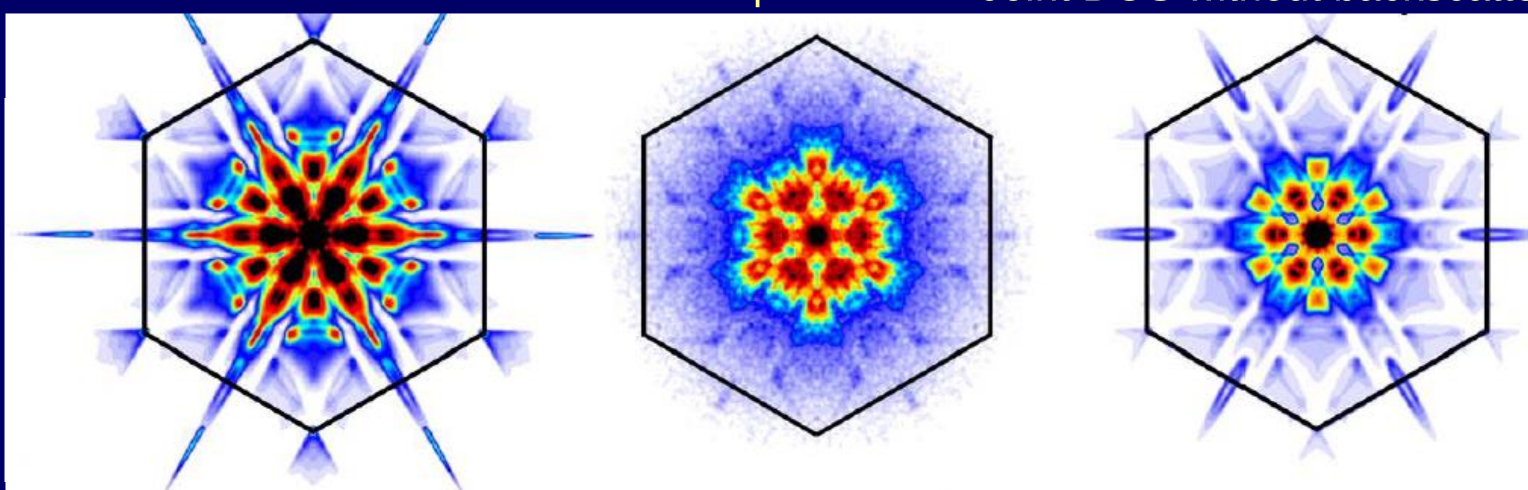
Li et al., Rev. Mod. Phys 83, 1057 (11)



Fourier transform

STM map of standing electron waves

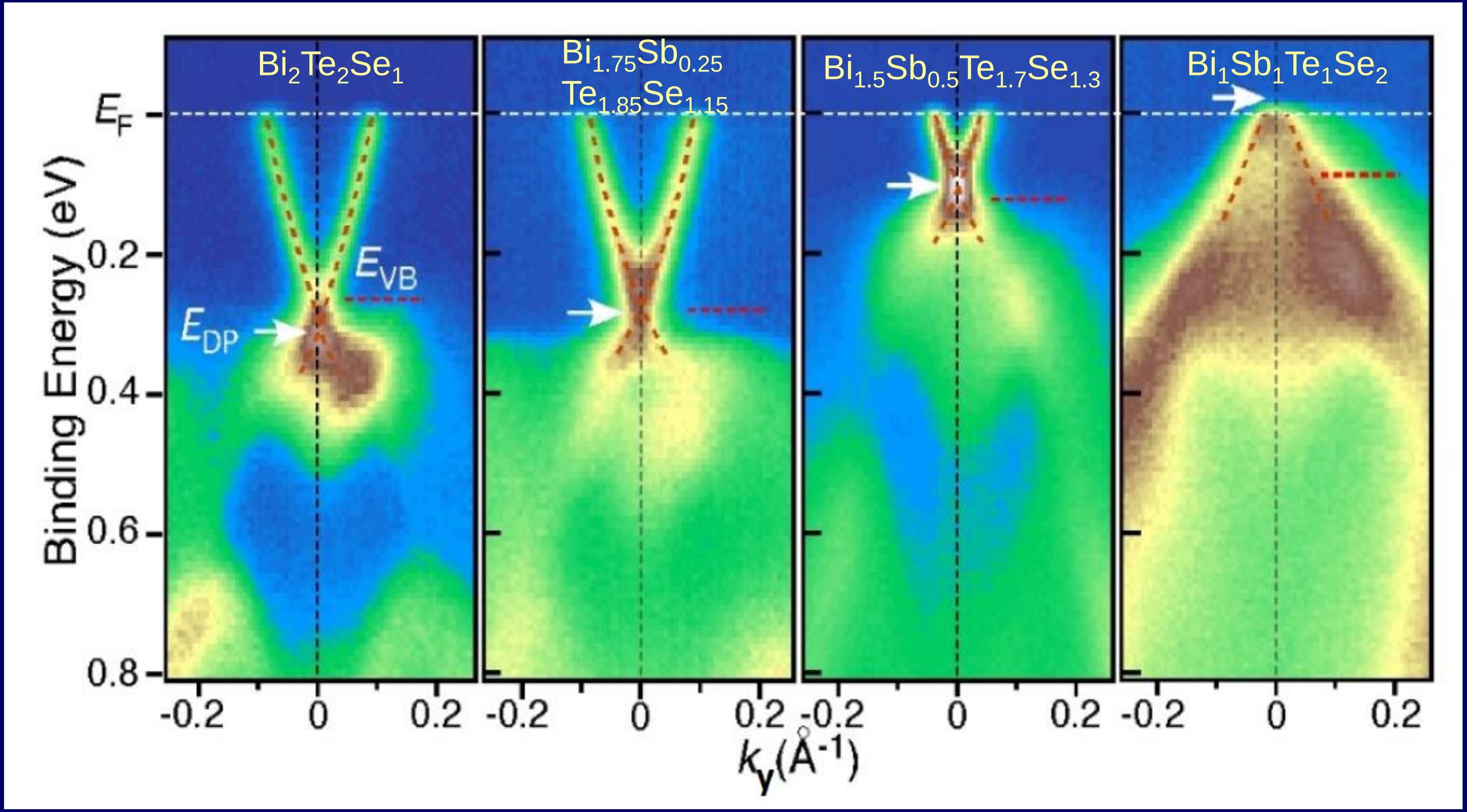
Joint DOS from ARPES | Experiment | Joint DOS without backscatter



Roushan et al. Nature 460, 1106 (09)

3D TI: tuning $E_F = E_D$

Mixing Bi_2Se_3 and Sb_2Te_3

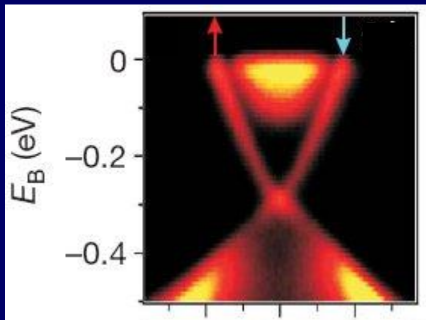


⇒ towards devices

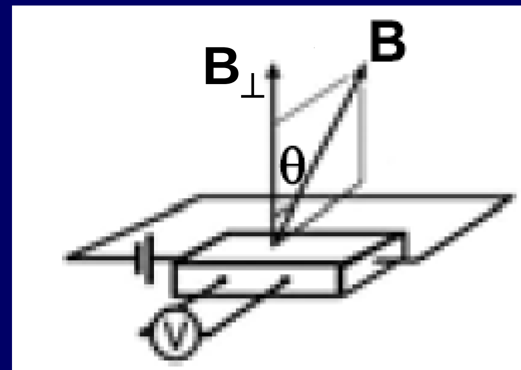
Y. Ando, J. Phys. Soc. Jap. 82, 102001 (13)

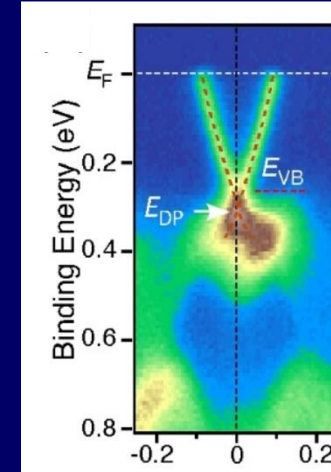
ARPES data

3D TI: magnetotransport

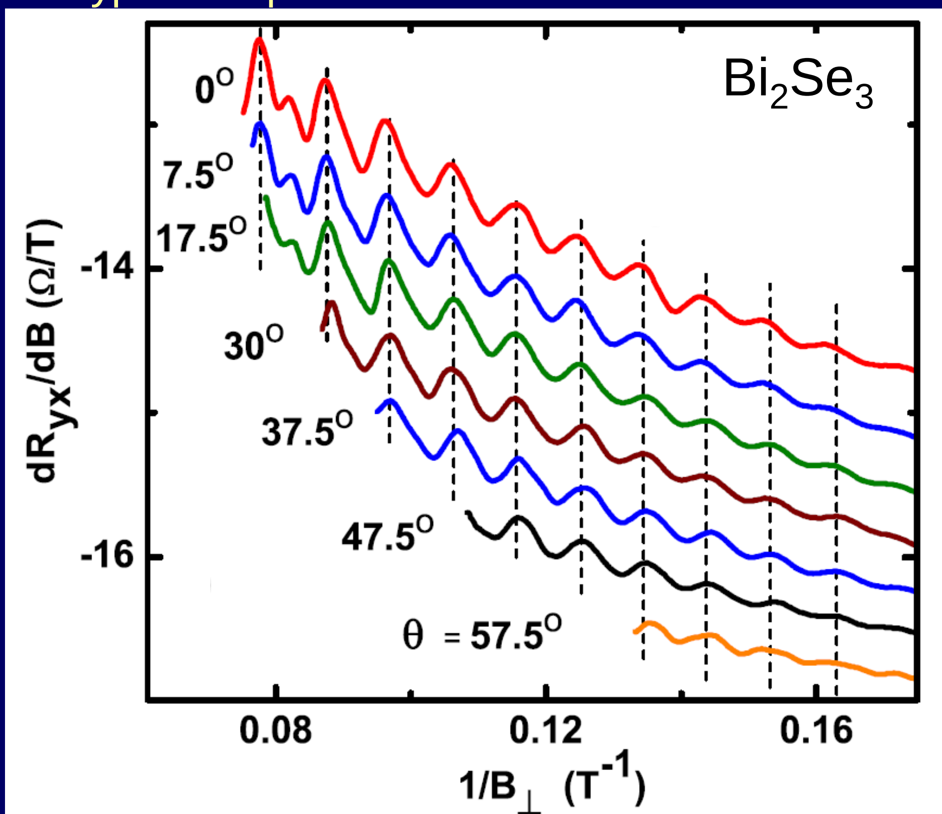


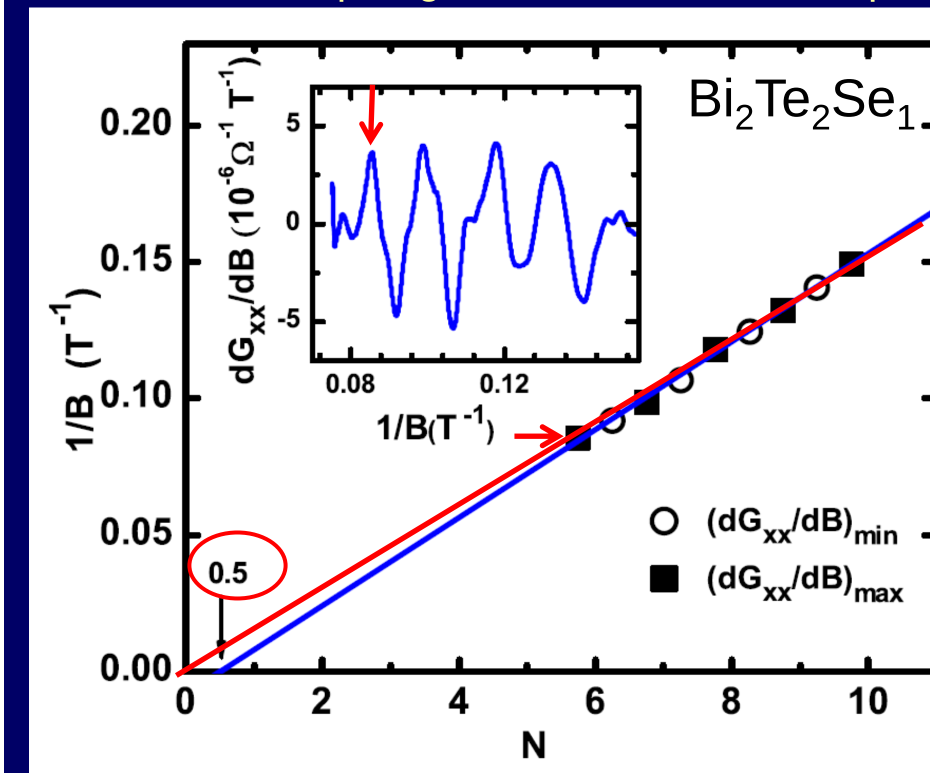
2D type transport





Topological surface state transport



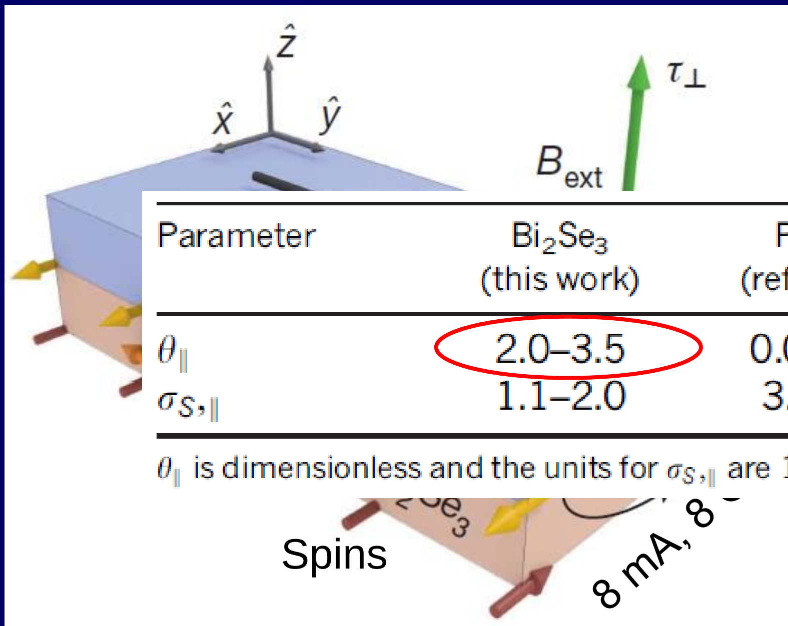


phase factor of oscillations due to Berry phase

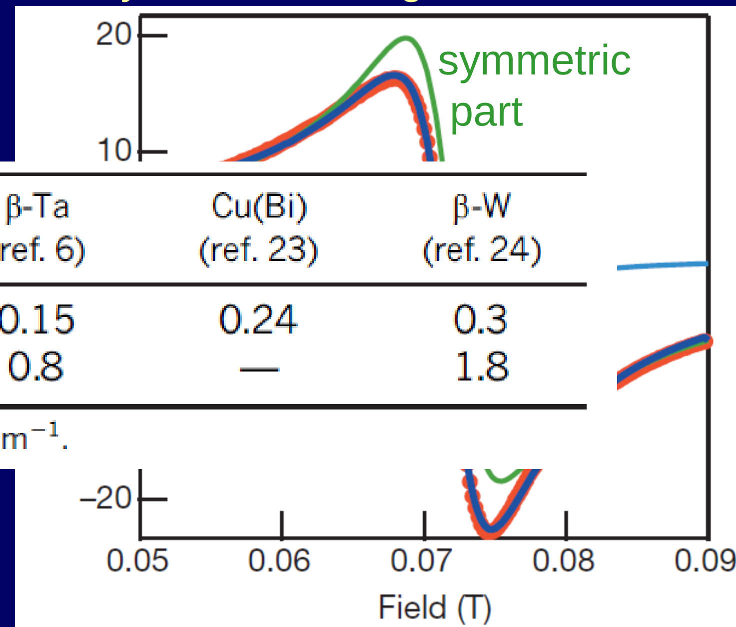
Y. Ando, J. Phys. Soc. Jap. 82, 102001 (13)

3D TI spin transport

Melnik et al., Nature 511, 449 (14)



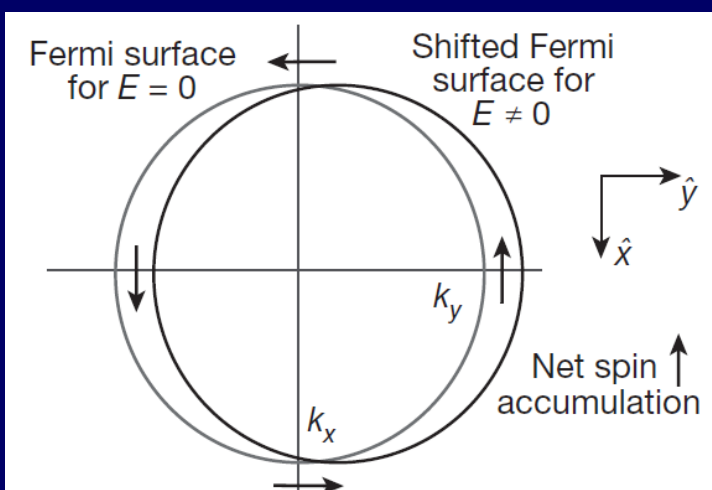
analysis of ferromagnetic resonance



Parameter	Bi_2Se_3 (this work)	Pt (ref. 4)	β-Ta (ref. 6)	Cu(Bi) (ref. 23)	β-W (ref. 24)
$\theta_\parallel$	2.0–3.5	0.08	0.15	0.24	0.3
$\sigma_{S,\parallel}$	1.1–2.0	3.4	0.8	—	1.8

$\theta_\parallel$ is dimensionless and the units for $\sigma_{S,\parallel}$ are $10^5\hbar/2e\,\Omega^{-1}\,\mathrm{m}^{-1}$.

Spin accumulation at interface induces torque τ on ferromagnet



fit to equation

$$\frac{\mathrm{d}\hat{m}}{\mathrm{d}t} = -\gamma\hat{m}\times\left(\vec{B}_{\mathrm{ext}} - \mu_0 M_{\mathrm{eff}} m_z \hat{z}\right) + \alpha\hat{m}\times\frac{\mathrm{d}\hat{m}}{\mathrm{d}t} + \gamma\tau_\parallel\frac{\hat{m}\times(\hat{x}\times\hat{m})}{|\hat{x}\times\hat{m}|} + \gamma\tau_\perp\frac{\hat{x}\times\hat{m}}{|\hat{x}\times\hat{m}|}$$

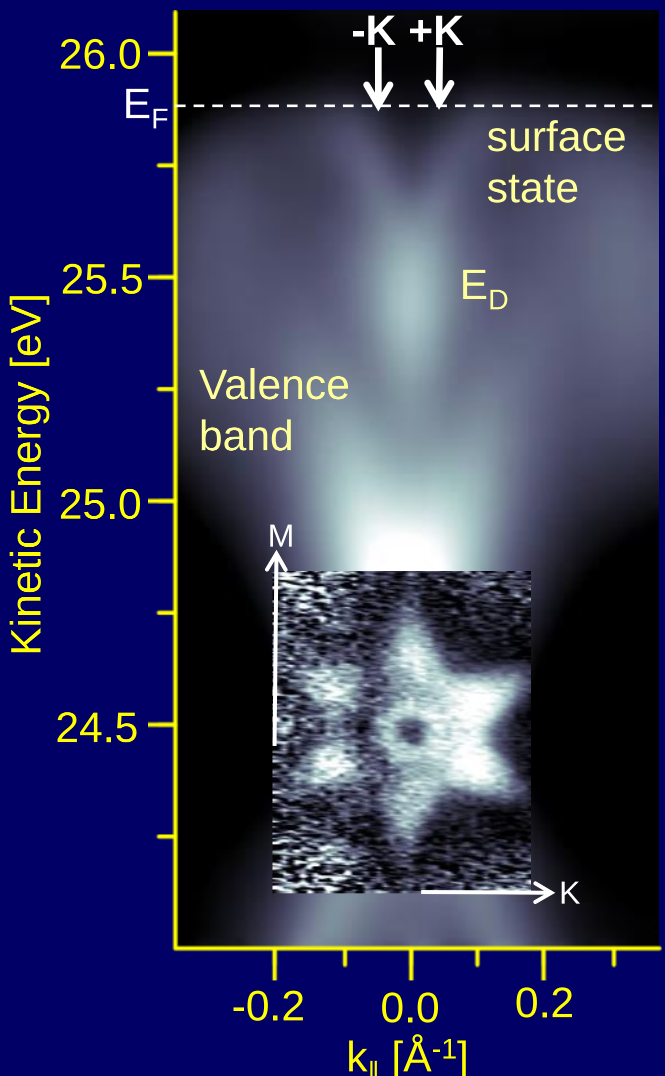
torque by spin accumulation

$$\hat{\theta} = \frac{\hat{T}}{j_y}\frac{2e}{\hbar}$$

spin torque per current density

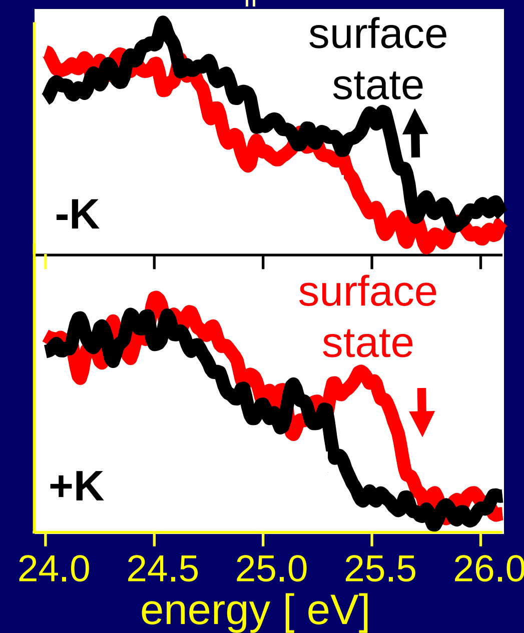
Towards switchable Topological Insulators

crystalline $Ge_2Sb_2Te_5$
$h\nu$: 30 eV

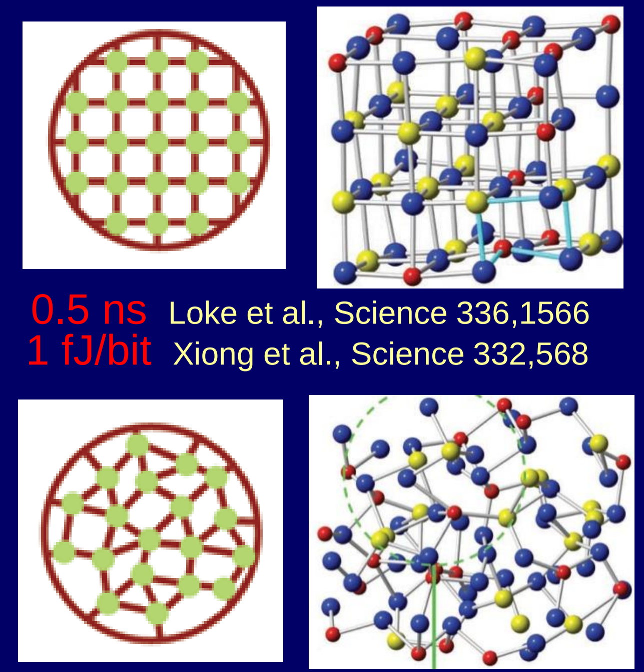


APL 103, 243109 (13)

Spin ARPES
perp $k_{||}$, in plane

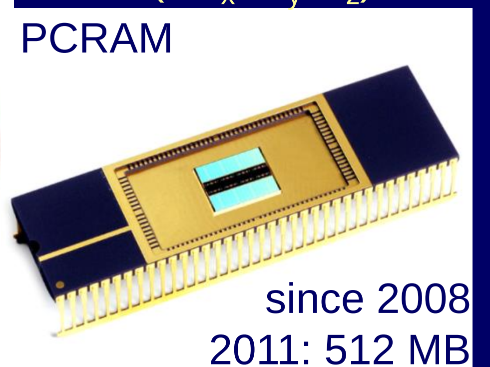


conducting



Loke et al., Science 336,1566
Xiong et al., Science 332,568

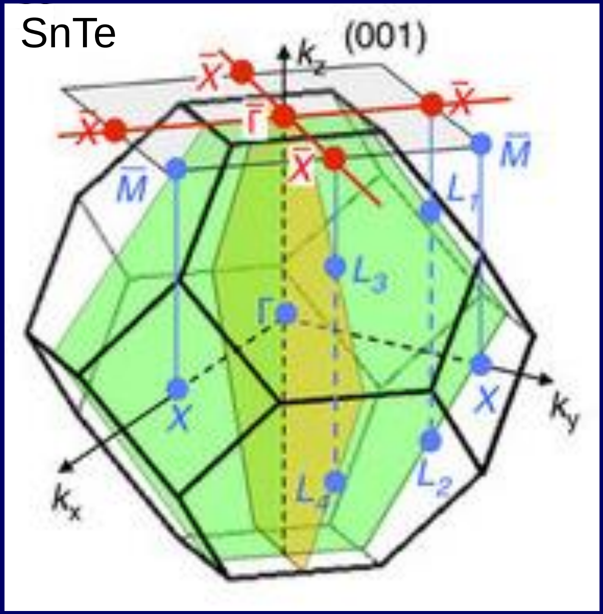
insulating
Phase change materials ($Ge_xSb_yTe_z$)



Hsieh et al., Nature Com. 3, 982 (12)

Topological Crystalline Insulators

Idea: use point group symmetries in Brillouin zone



4 non-equivalent TRIMs at L1-L4 with inverted band gap = trivial Z2

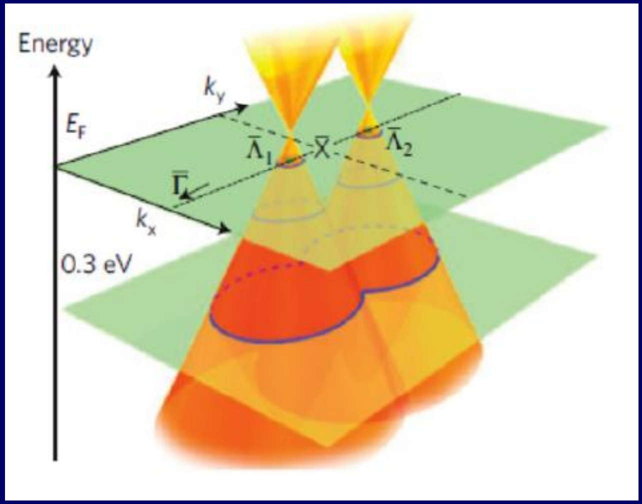
L3, L4 on mirror plane:

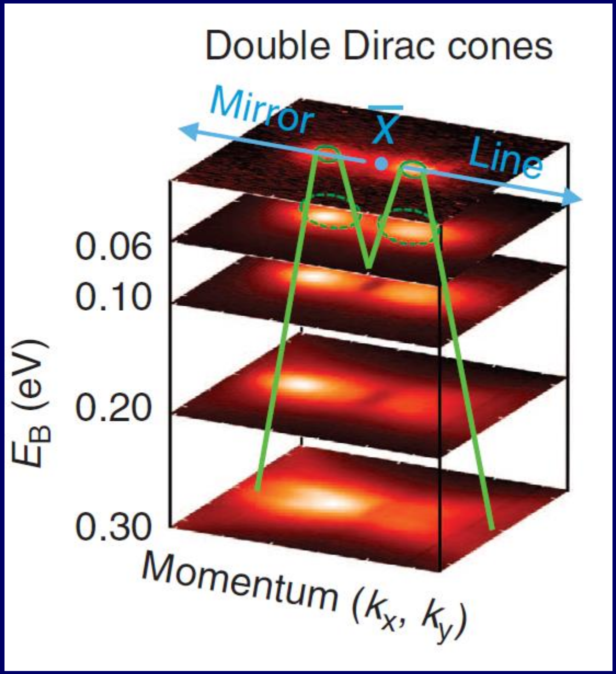
classify mirror parities: $n_+ - n_-$

Γ: +1   L3, L4: -1

⇒ surface states for any surface with mirror symmetry between $\bar{\Gamma}$ and $\bar{X}$

DFT: band inversion at L removed in PbTe





ARPES $Pb_{0.6}Sn_{0.4}Te$

Xu et al., Nature Com. 3, 1192 (12)

Even more general ?

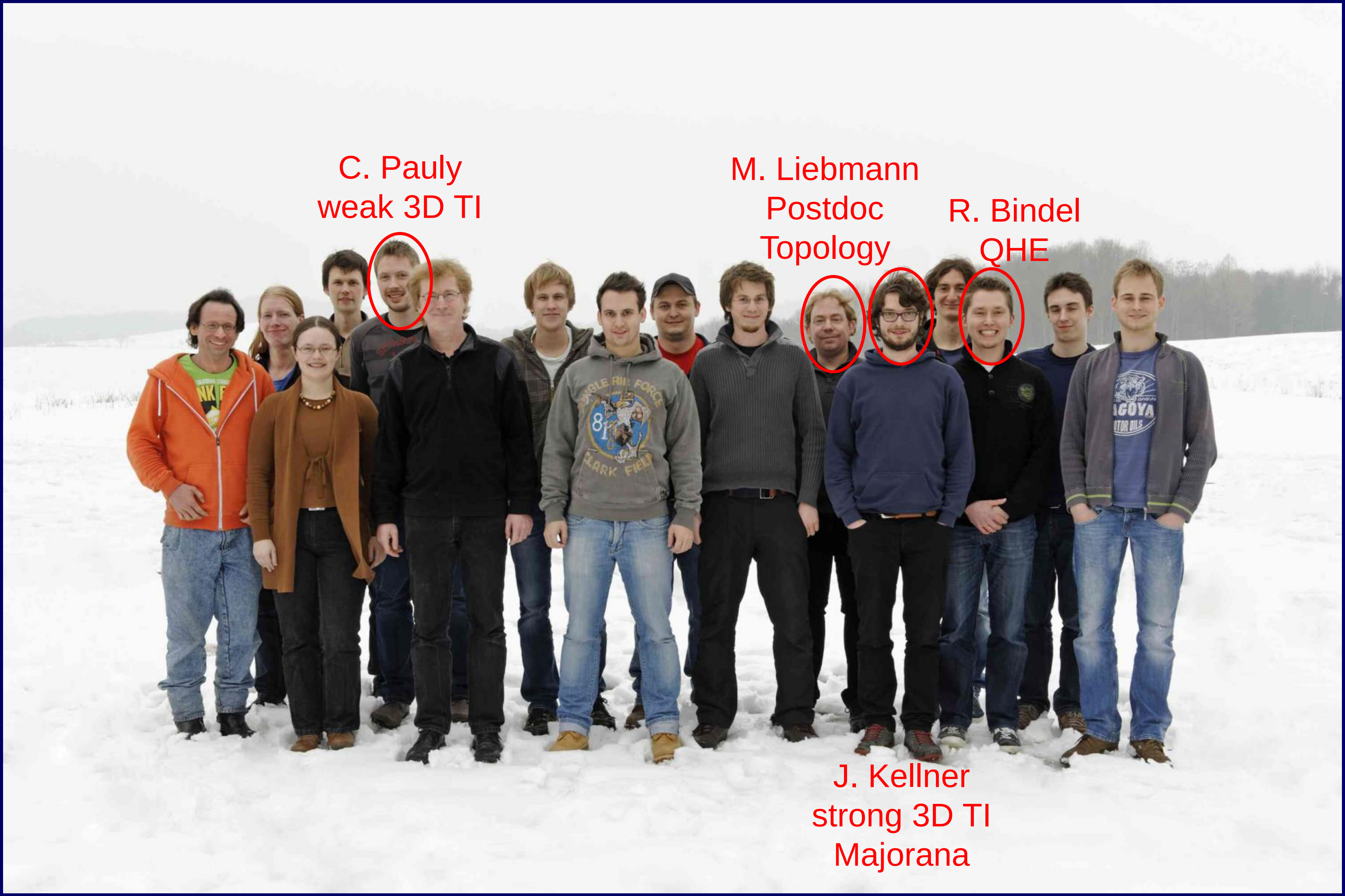
Towards a periodic table of topology

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
Chiral	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$	-	$\mathbb{Z}$
(sublattice)	BDI (chiral orthogonal)	+1	+1	1	$\mathbb{Z}$	-	-
	CII (chiral symplectic)	−1	−1	1	$\mathbb{Z}$	-	$\mathbb{Z}_2$
BdG	D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	-
	C	0	−1	0	-	$\mathbb{Z}$	-
	DIII	−1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	+1	−1	1	-	-	$\mathbb{Z}$

Schnyder et al.
PRL 78, 195125

AZ class	Space of projectors in momentum space	BL class	$N_f^{\min}$	Fermionic replica NLσM target space	Topological or WZW term
A	$\{Q(k) \in G_{m,m+n}(\mathbb{C})\}$	**0**	1	$U(2N)/U(N)\times U(N)$	Pruisken
AI	$\{Q(k) \in G_{m,m+n}(\mathbb{C}) \mid Q(k)^* = Q(-k)\}$	$\mathbf{4}_+$	2	$Sp(2N)/Sp(N)\times Sp(N)$	N/A
AII	$\{Q(k) \in G_{2m,2(m+n)}(\mathbb{C}) \mid (i\sigma_y)Q(k)^*(-i\sigma_y) = Q(-k)\}$	$\mathbf{3}_+$	1	$O(2N)/O(N)\times O(N)$	$\mathbb{Z}_2$
AIII	$\{q(k) \in U(m)\}$	**1** or **2**	1 or 2	$U(N)\times U(N)/U(N)$	WZW
BDI	$\{q(k) \in U(m) \mid q(k)^* = q(-k)\}$	$\mathbf{9}_+$	2	$U(2N)/Sp(N)$	N/A
CII	$\{q(k) \in U(2m) \mid (i\sigma_y)q(k)^*(-i\sigma_y) = q(-k)\}$	$\mathbf{9}_-$	2	$U(2N)/O(2N)$	$\mathbb{Z}_2$
D	$\{Q(k) \in G_{m,2m}(\mathbb{C}) \mid \tau_x Q(k)^* \tau_x = -Q(-k)\}$	$\mathbf{3}_-$	1	$O(2N)/U(N)$	Pruisken
C	$\{Q(k) \in G_{m,2m}(\mathbb{C}) \mid \tau_y Q(k)^* \tau_y = -Q(-k)\}$	$\mathbf{4}_-$	2	$Sp(N)/U(N)$	Pruisken
DIII	$\{q(k) \in U(2m) \mid q(k)^T = -q(-k)\}$	**5** or **7**	1 or 2	$O(2N)\times O(2N)/O(2N)$	WZW
CI	$\{q(k) \in U(m) \mid q(k)^T = q(-k)\}$	**6** or **8**	2 or 4	$Sp(N)\times Sp(N)/Sp(N)$	WZW

People


C. Pauly
weak 3D TI
M. Liebmann
Postdoc
Topology
R. Bindel
QHE
J. Kellner
strong 3D TI
Majorana

Summary

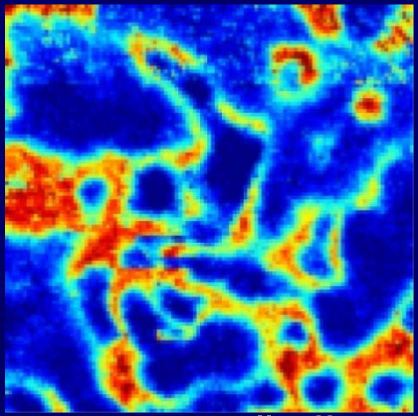
Topological indices:

Integer bulk property requiring robust non-trivial transversal conductivity which implies boundary states at E_F

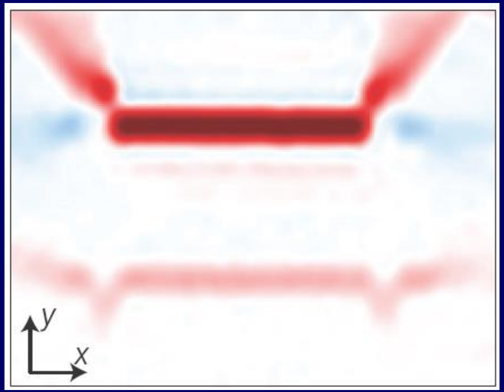
Experimentally realized:

- Quantum Hall effect (80's): GaAs, Si, Graphene, …
- 2D Topological insulator: HgTe, InAs/GaSb
- Quantum anomolous Hall effect: BiCrSbTe
- Weak 3D topological insulator: BiRhI
- **Strong 3D topological insulator** (many examples, mostly SO, but also Kondo ?)
- Topological crystalline insulators: SnTe

…



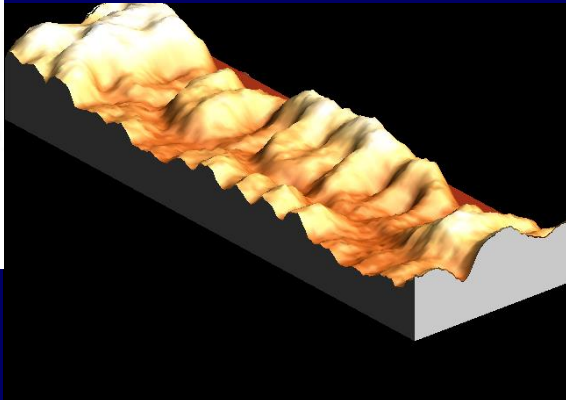
Quantum Hall effect



2D TI

3D TI: strong

3D TI: weak



Hasan et al., Rev. Mod. Phys 82, 3045 (10)
Li et al., Rev. Mod. Phys 83, 1057 (11)
Y. Ando, J. Phys. Soc. Jap. 82, 102001 (13)