Introduction to topology in electronic structure of crystalline solids

Tomáš Rauch

IFTO, FSU Jena

Schedule

- 24.03. Introduction into topological insulators
- 14.04. Topological insulators in two and three dimensions
- 21.04. Calculation of topological invariants of realistic materials
- 28.04. Role of spin-orbit coupling, band inversions and experimental evidence
- 05.04. Further (theoretical) concepts
- TBA Topological metals and higher-order topological insulators
- TBA Applications / Unanswered topics?

Literature

- D. Vanderbilt, Berry phases in electronic structure theory
- B. A. Bernevig, Topological insulators and topological superconductors
- J. K. Asboth, L. Oroszlany, A. Pályi, A short course on topological insulators

Topological insulators with time-reversal symmetry

topological invariant: $\nu \in \{0, 1\}$

- in presence of inversion symmetry[1]:
  - ξ_{2m} parity of occupied degenerate pairs of states at d TRIMs

$$(-1)^{\nu} = \prod_{i=1}^{d} \delta_i \text{ with } \delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

  - 2D: $d = 4$
  - 3D: $d = 8$

[1] Fu and Kane, PRB **76**, 045302(2007)
[2] Iraola *et al.*, arXiv:2009.01764

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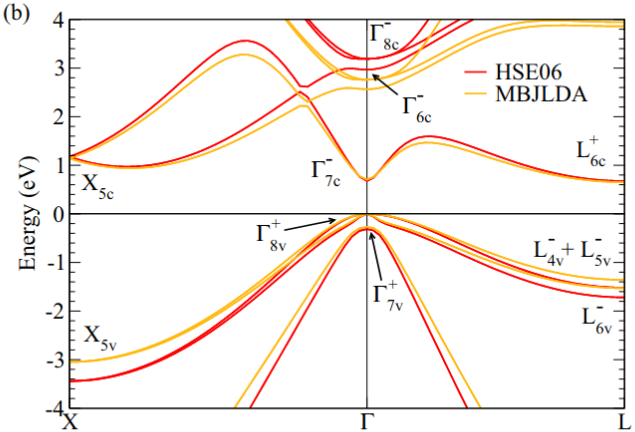
- Ge^2 (diamond structure)



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  - VASP input: WAVECAR, POSCAR
  - lists symmetry operations of the SG

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$\pi/2$ rotation: `# 14`

```
 rotation :   | 0 0 -1 |
              | 0 -1 0 |
              | -1 0 0 |
 spinor :   | 0.000-0.707j -0.000+0.707j   |
            | 0.000+0.707j 0.000+0.707j    |
translation :  [ 0.000000 0.000000 0.000000 ]
axis:  [-0.707 0.  0.707]; angle = 1 pi, inversion:  False
```

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inversion: # 25

```
 rotation :   | -1 0 0 |
              | 0 -1 0 |
              | 0 0 -1 |
 spinor :   | 1.000+0.000j 0.000+0.000j |
            | 0.000+0.000j 1.000+0.000j |
translation :  [ 0.000000 0.000000 0.000000 ]
axis:[-0.078 -0.078 0.993]; angle=0, inversion:  True
```

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  - lists symmetry operations of the SG
  - gives characters of the IrReps and labels

Γ point:

```
k-point 1 :[0.  0.  0.]
number of irreps = 3
  Energy    |  multiplicity  |     irreps     |  sym.  operations
            |                |                |         25
 -8.7801    |       2        |   -GM6(1.0)    |       2.0000
  3.5557    |       2        |   -GM7(1.0)    |       2.0000
  3.8268    |       4        |  -GM10(1.0)    |       4.0000
inversion is # 25
number of inversions-odd Kramers pairs :  0
```

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L point:

```
k-point 8 :[0.5 0.5 0.5]
number of irreps = 7
 Energy   multiplicity         irreps          sym.  operations
                                                       25
 -6.7132       2              -L9(1.0)               -2.0000
 -3.5762       2              -L8(1.0)                2.0000
  2.3138       2              -L9(1.0)               -2.0000
  2.4872       2         -L6(1.0), -L7(1.0)          -2.0000
inversion is # 25
number of inversions-odd Kramers pairs :  3
```

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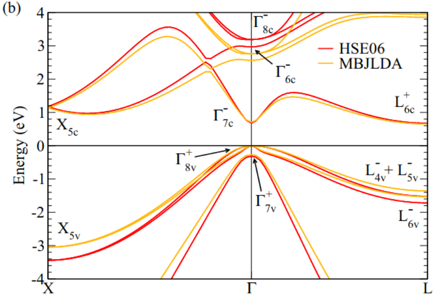
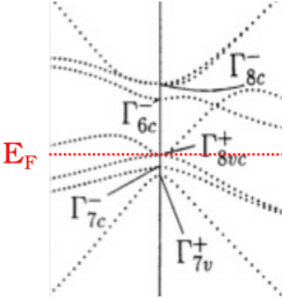
Topological insulators with time-reversal symmetry

band inversion:

- in presence of inversion symmetry[3]:
- Ge[4] vs. Sn[5] (diamond structure)





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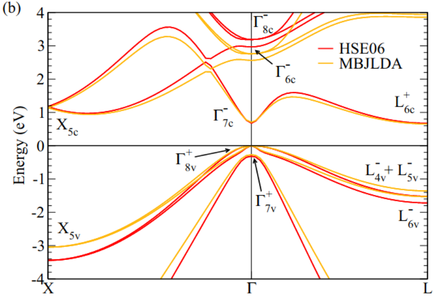

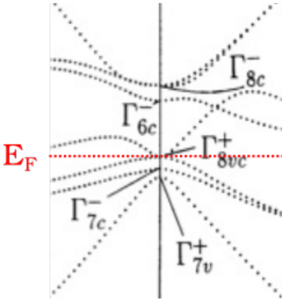

- switching of the IrReps of the occupied bands

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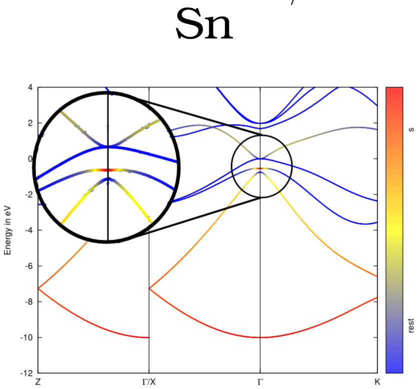
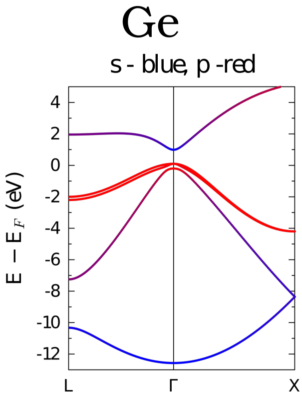
band inversion:

- in presence of inversion symmetry[3]:
- switching of the IrReps of the occupied bands
- often visible from atomic / orbital character





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band inversion:

- important ingredient: **spin-orbit coupling** (SOC)

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- SOC preserves time-reversal:
  - spherically symmetric ionic potentials: $V_{\mathrm{SO}}(\mathbf{r}) = \lambda(\mathbf{r})\boldsymbol{l} \cdot \boldsymbol{s}$
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  - $\boldsymbol{s}$ ...spin
  - $\boldsymbol{l}$ ...orbital angular momentum
  - time-reversal:

$$t \to -t$$

$$\boldsymbol{s} \to -\boldsymbol{s}$$

$$\boldsymbol{l} \to -\boldsymbol{l}$$

$$\boldsymbol{l}\cdot\boldsymbol{s} \to (-\boldsymbol{l})\cdot(-\boldsymbol{s}) = \boldsymbol{l}\cdot\boldsymbol{s}$$

Topological insulators with time-reversal symmetry

band inversion:

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- **role 1**: causing band inversion

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- example: Bi_2Te_3
  - f ...fraction of real SOC
  - yellow: Te-p_z character

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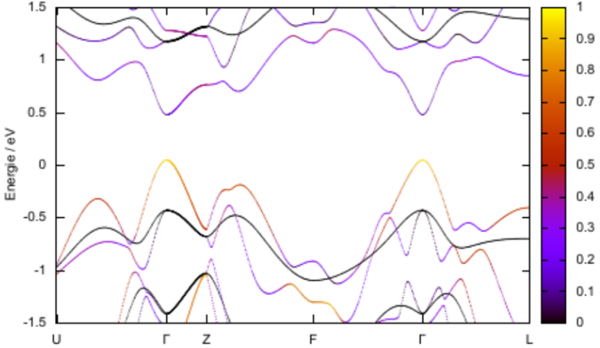

(a) $f = 0.0,\ \nu_0 = 0$

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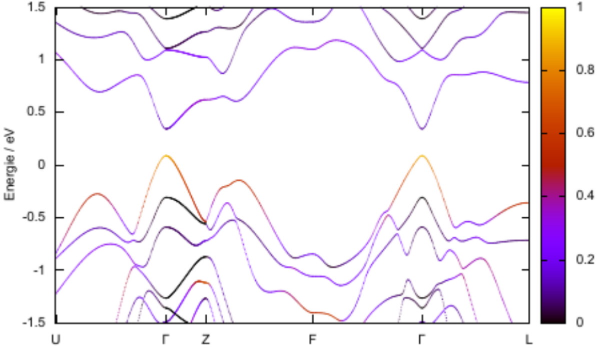

(c) $f = 0.4,\ \nu_0 = 0$

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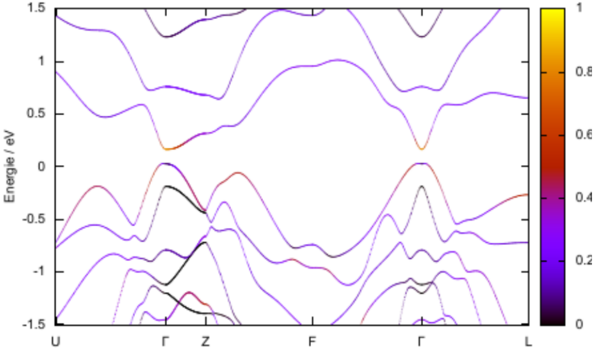

(e) $f = 0.8,\ \nu_0 = 1$

Topological insulators with time-reversal symmetry

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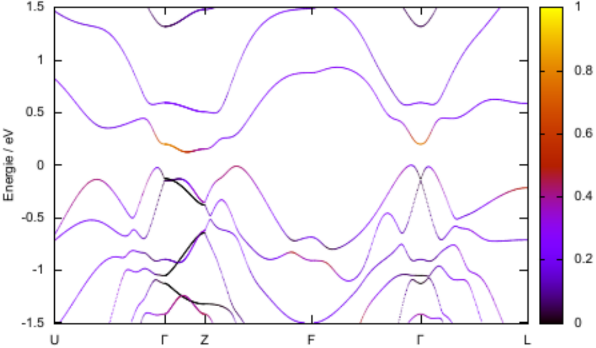
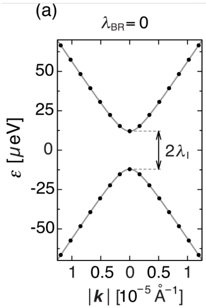


(f) $f = 1.0$, $\nu_0 = 1$

Topological insulators with time-reversal symmetry

band inversion:

- important ingredient: **spin-orbit coupling** (SOC)
- **role 1**: causing band inversion
- example: Bi_2Te_3
- **role 2**: opening the band gap
- example: graphene[4] ($E_g \approx 24\mu$eV)



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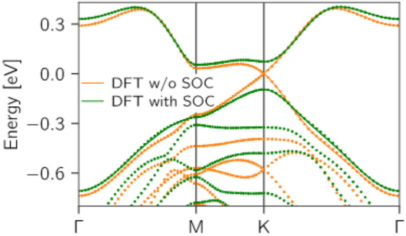

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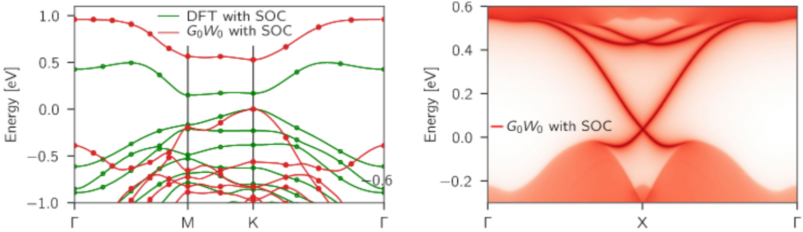

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Topological insulators with time-reversal symmetry

band inversion:

- often caused by other effects than SOC:
  - e.g. relativistic Darwin term, strain,...[6]

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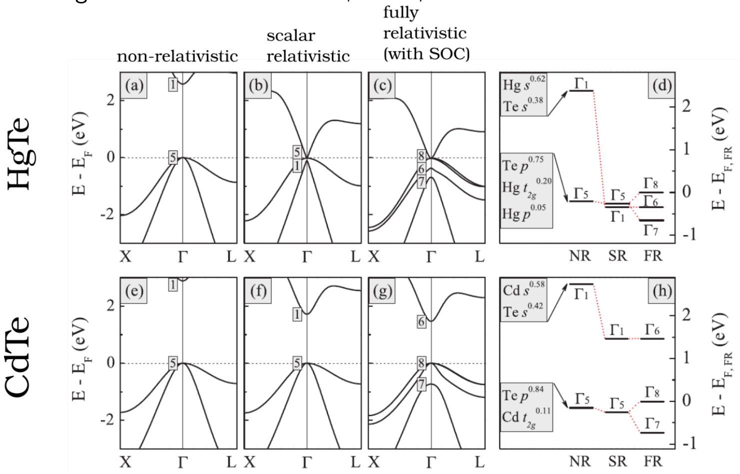

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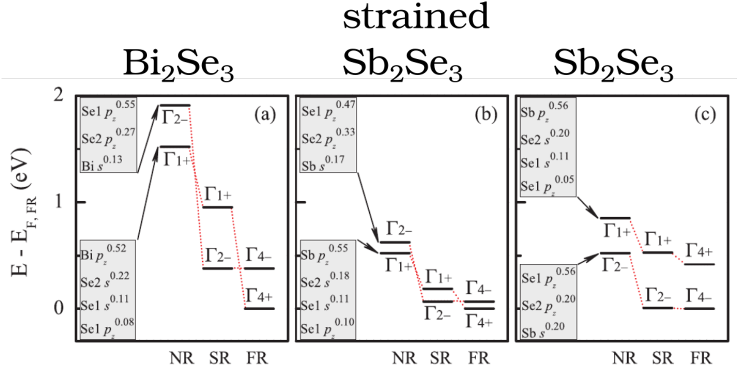

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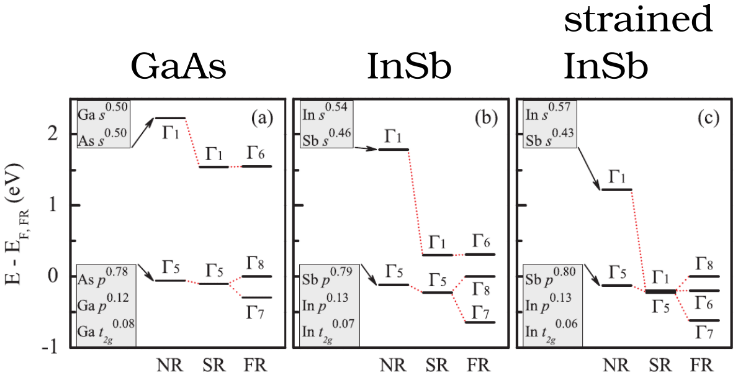

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Topological insulators with time-reversal symmetry

band inversion:

- often caused by other effects than SOC:
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- role of SOC often "just" to open band gaps (avoided crossings)
  - band gaps of TIs often limited by the SOC strength

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Experimental evidence

1D transport at the edge of 2D TIs

- MoS_2
  - 2H phase - normal insulator, $\nu = 0$
  - 1T' phase - topological insulator, $\nu = 1$

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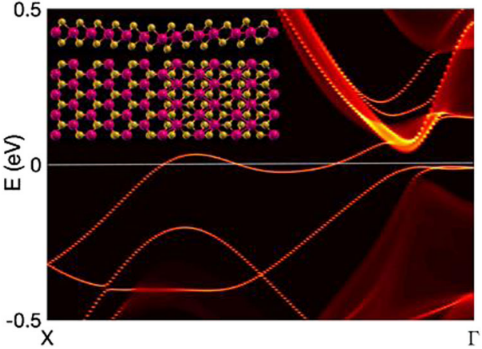

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  - 1T' phase by laser irradiation[7]

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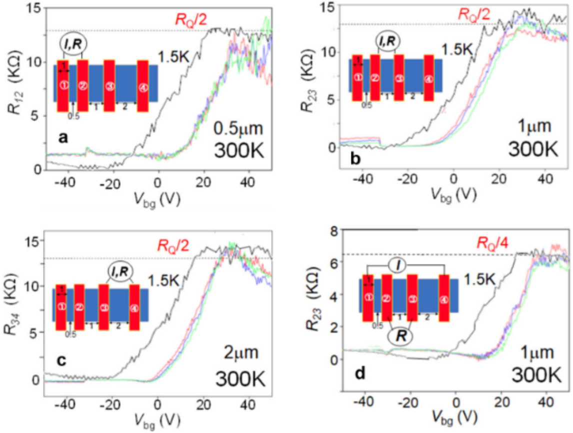
Experimental evidence

1D transport at the edge of 2D TIs

- MoS_2
  - two- and four-probe resistance measurements[7]
  - theoretical values from Landauer-Büttiker formalism



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STM at 1D edge of 2D TIs

- ML jacutingaite (Pt_2HgSe_3)[8]
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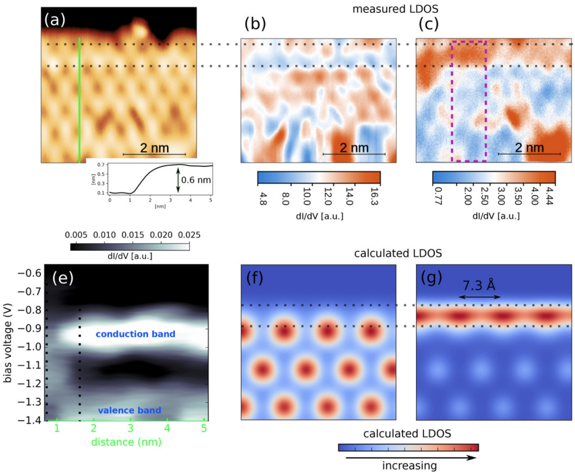

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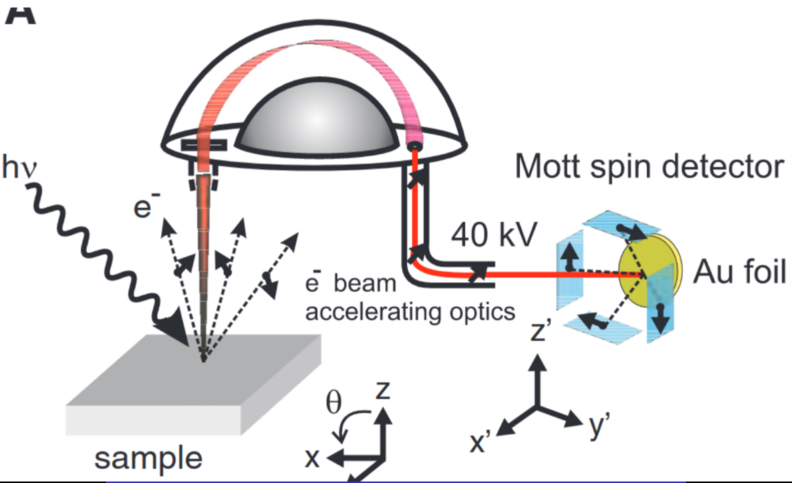
Spin- and angle-resolved photoemission spectroscopy



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Spin- and angle-resolved photoemission spectroscopy

- band structure visualization

[9] Hsieh *et al.*, Science **323**, 919 (2009)
[10] Chen *et al.*, Science **329**, 659 (2010)

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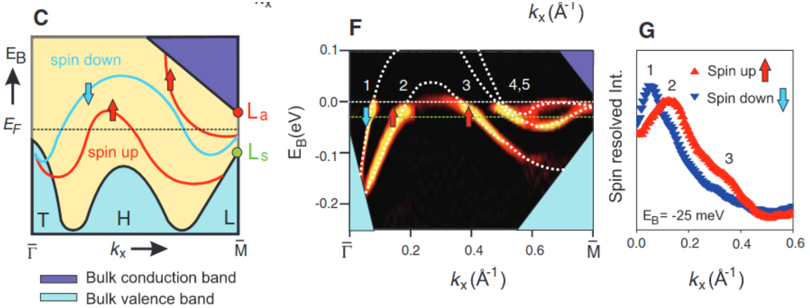
- $Bi_{1-x}Sb_x$[9]



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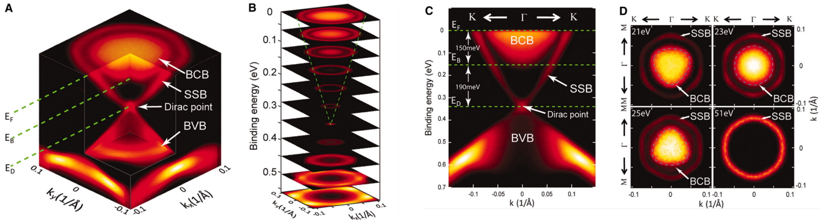

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Experimental evidence

Surface state Landau levels spectroscopy

[11] Cheng *et al.*, PRL **105**, 076801 (2010)

Experimental evidence

Surface state Landau levels spectroscopy

- Bi_2Se_3[11]
  - magnetic field perpendicular to the surface
  - dI/dV from STM, while scanning the chemical potential

[11] Cheng *et al.*, PRL **105**, 076801 (2010)

Experimental evidence

Surface state Landau levels spectroscopy

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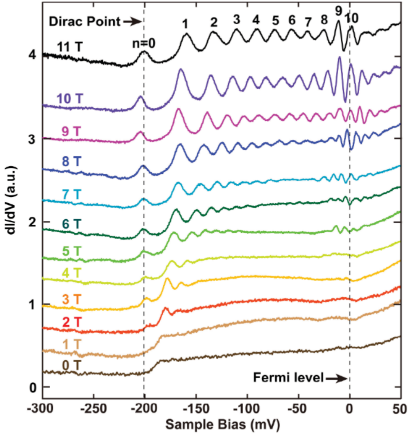

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Surface state Landau levels spectroscopy

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  - LLs of massless Dirac fermions: $E_n \propto \sqrt{|n|B}$
  - LLs of free electrons: $E_n \propto nB$, $n = 0, \pm 1, \ldots$

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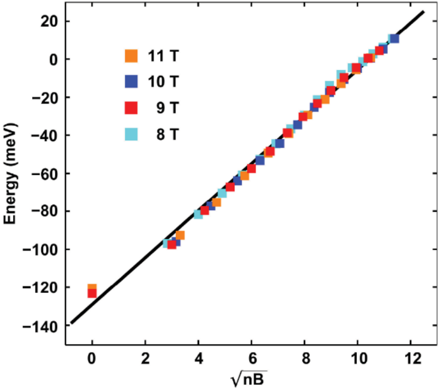

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$$\alpha_{ij} = \left.\frac{\partial P_i}{\partial \mathcal{B}_j}\right|_{\boldsymbol{\mathcal{E}}=0} = \left.\frac{\partial M_j}{\partial \mathcal{E}_i}\right|_{\boldsymbol{\mathcal{B}}=0}$$

orbital frozen-ion part

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  orbital frozen-ion part
- TRS: $\boldsymbol{\mathcal{B}} \to -\boldsymbol{\mathcal{B}}$ or $\mathbf{M} \to -\mathbf{M} \Rightarrow \alpha \to -\alpha$
  $\Rightarrow \alpha = 0$ with TRS?

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- isotropic part of α in periodic systems is multivalued:

$$\alpha_{\mathrm{iso}} = \alpha_{\mathrm{iso}}^{\mathrm{b}ulk} \mod \frac{e^2}{h}$$

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- together with $\alpha = -\alpha$ (TRS):

$$\alpha_{\text{iso}} = \begin{cases} 0 \mod \frac{e^2}{h} & \dots\text{trivial} \\ \frac{1}{2}\frac{e^2}{h} \mod \frac{e^2}{h} & \dots\text{non-trivial} \end{cases}$$

TIs and magnetoelectric coupling

Surface theorem

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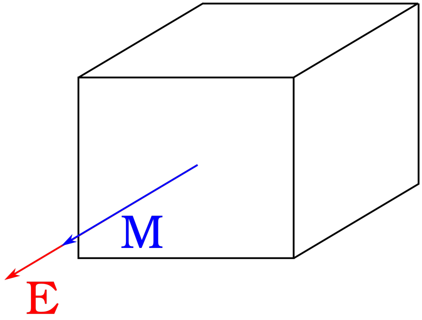
- isotropic magnetoelectric (ME) insulator: $\mathbf{M} = \alpha_{\text{iso}} \boldsymbol{\mathcal{E}}$



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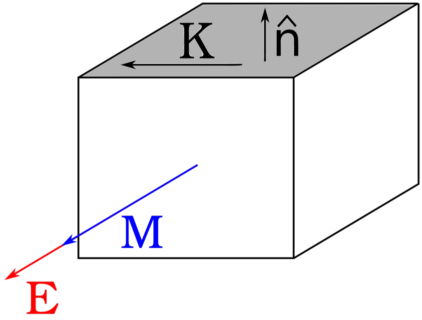
- surface current $\mathbf{K} = \mathbf{M} \times \hat{\mathbf{n}}$



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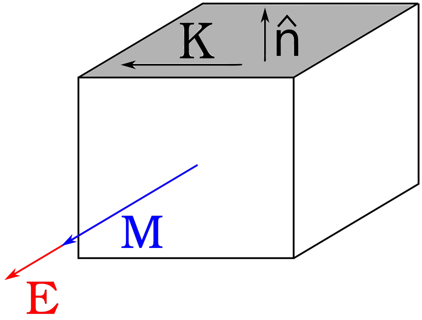

[12] S. Coh *et al.*, PRB **83**, 085108 (2011)

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$$\sigma_{\mathrm{AH}}^{\mathrm{surf}} = -\alpha_{\mathrm{iso}} + m\frac{e^2}{h} + \sigma_{E_F}$$

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- consequence for a TI with gapped TSS (broken TRS on the surface):

$$\sigma_{\text{AH}}^{\text{surf}} = \left(m - \frac{1}{2}\right)\frac{e^2}{h}$$

$\rightarrow$ half-quantized AHC!

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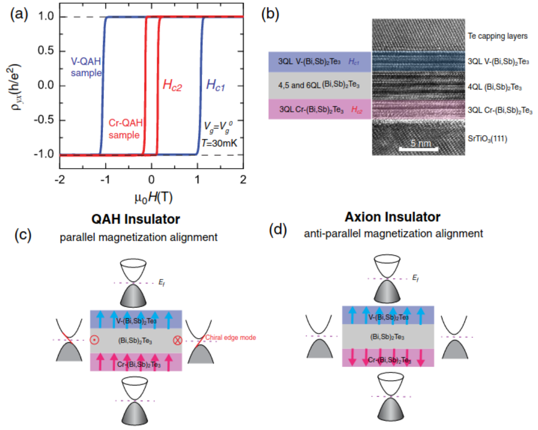
Experimental evidence

Half-quantized surface AHC

- $(Bi,Sb)_2Te_3$, ferromagnetic surface layers[13] (top: V, bottom: Cr)
  - ferromagnetic surface layers: QAHI

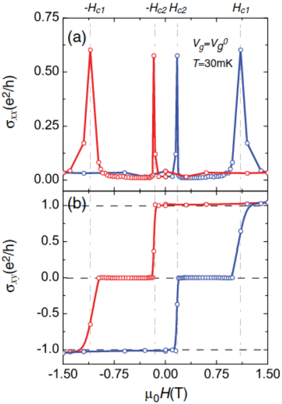


[13] Xiao *et al.*, PRL **120**, 056801 (2018)

Experimental evidence

Half-quantized surface AHC

- $(Bi,Sb)_2Te_3$, ferromagnetic surface layers[13] (top: V, bottom: Cr)
  - ferromagnetic surface layers: QAHI
  - both surfaces measured: $\sigma_{xy} = (m_{\mathrm{top}} - 1/2 + m_{\mathrm{down}} - 1/2)\ e^2/h$



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Conclusion

- spin-orbit coupling
- band inversion
- experiments

Following seminars:

1. theory: (hybrid) Wannier functions
2. topological metals, Weyl-, Dirac-, (Majorana-)fermions; higher-order TIs?
3. applications?