Introduction to topology in electronic structure of crystalline solids

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Schedule

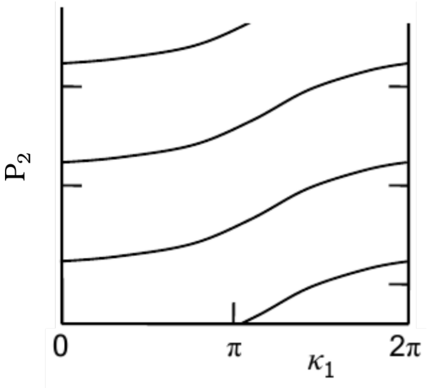
- 24.03. Introduction into topological insulators
- 14.04. Topological insulators in two and three dimensions
- 21.04. Calculation of topological invariants of realistic materials
- 28.04. Further concepts related to topological insulators
- TBA Topological metals and higher-order topological insulators
- TBA Applications
- TBA Unanswered topics?

Literature

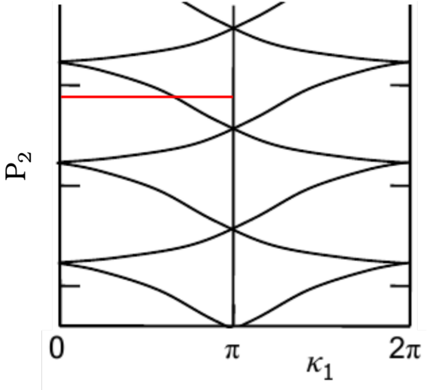
- D. Vanderbilt, Berry phases in electronic structure theory
- B. A. Bernevig, Topological insulators and topological superconductors
- J. K. Asboth, L. Oroszlany, A. Pályi, A short course on topological insulators

2D topological insulators

- broken time-reversal symmetry
- Quantum-Hall (Chern) insulator
- (anomalous) quantum Hall effect



- with time-reversal symmetry
- Quantum-Spin-Hall ($\mathcal{Z}_2$) ins.
- Spin Hall effect



Practical calculation of the $\mathcal{Z}_2$ topological invariant (2D)

- polarization pumping (ΔP_2 for $k_1 : 0 \to 2\pi/a$)

[1] Kane and Mele, PRL **95**, 146802 (2005)
[2] Fu and Kane, PRB **74**, 195312 (2006)
[3] Fu and Kane, PRB **76**, 045302(2007)

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- properties of the Pfaffian[1] $\mathrm{Pf}\,[w(\boldsymbol{k})]$ with $w_{nm}(\boldsymbol{k}) = \langle u_{n,-\boldsymbol{k}} |\, \theta \,| u_{m,\boldsymbol{k}} \rangle$
  - $\mathrm{Pf}\,[A]^2 = \det[A]$
  - 2 occupied bands: $\mathrm{Pf}\,[w(\boldsymbol{k})] = \; w_{12}$

$$(-1)^{\nu} = \prod_{i=1}^{4} \frac{\sqrt{\det[w(\Gamma_i)]}}{\mathrm{Pf}[w(\Gamma_i)]} \qquad \Gamma_i \ldots \mathrm{TRIMs}$$

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- Fu-Kane formula[2]

$$\nu = \frac{1}{2\pi} \left[\sum_{n}^{\mathrm{occ.}} \left\{ \oint_{\partial \frac{1}{2}\mathrm{BZ}} d\boldsymbol{k}\, \boldsymbol{A}_n(\boldsymbol{k}) - \int_{\frac{1}{2}\mathrm{BZ}} d^2\boldsymbol{k}\; \boldsymbol{\Omega}_n^z(\boldsymbol{k}) \right\} \right] \quad \mathrm{mod}\ 2$$

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- in presence of inversion symmetry[3]:
  - ξ_{2m} parity of occupied degenerate pairs of states at TRIMs

$$(-1)^\nu = \prod_{i=1}^{4} \delta_i \text{ with } \delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

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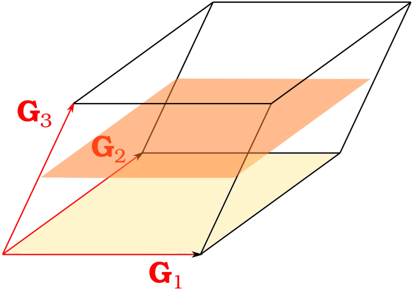
Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- 3D primitive reciprocal cell: six TR-invariant planes:
  $\left\{\boldsymbol{k} : \boldsymbol{k} = a_1\boldsymbol{G}_1 + a_2\boldsymbol{G}_2 + c\boldsymbol{G}_3 \mid a_1, a_2 \in (0,1),\ c \in \left\{0, \tfrac{1}{2}\right\}\right\}$ + cycl.



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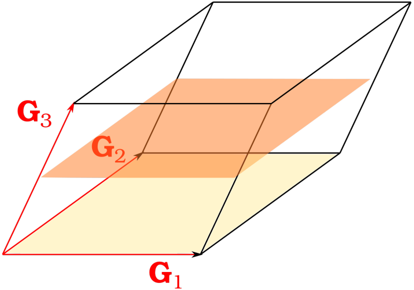

- six topological $\mathbb{Z}_2$ invariants protected by TR: $\nu_1, \tilde{\nu}_1, \nu_2, \tilde{\nu}_2, \nu_3, \tilde{\nu}_3$

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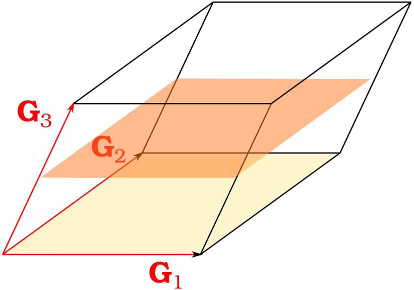

- six topological $\mathbb{Z}_2$ invariants protected by TR: $\nu_1, \tilde{\nu}_1, \nu_2, \tilde{\nu}_2, \nu_3, \tilde{\nu}_3$
- only four independent invariants: $(\nu_0; \nu_1\nu_2\nu_3)$
  - $\nu_0 = |\nu_1 - \tilde{\nu}_1| = |\nu_2 - \tilde{\nu}_2| = |\nu_3 - \tilde{\nu}_3|$
  - $(0; 000)$ trivial insulator
  - $(0; \nu_1\nu_2\nu_3)$ weak topological insulator ... stacked 2D TIs
  - $(1; \nu_1\nu_2\nu_3)$ strong topological insulators ... true 3D origin

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- in presence of inversion symmetry[4]:
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$$(-1)^{\nu} = \prod_{i=1}^{8} \delta_i \text{ with } \delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

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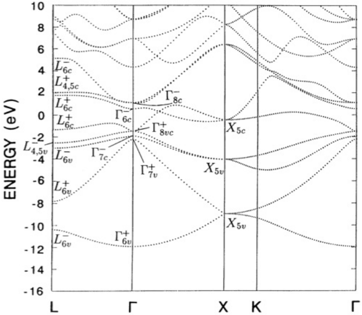
Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- α-Sn (diamond structure, strained)[4]



  - Γ (1x): (001) strain breaks degeneracy of Γ_8^+: Γ_6^+, Γ_7^+, Γ_7^-, Γ_8^+ $\Rightarrow \delta_\Gamma = -1$
  - X (3x): X_5 has parities $(+,+,-,-)$: X_5, X_5 $\Rightarrow \delta_X = +1$
  - L (4x): L_6^-, L_6^+, L_6^-, $L_{4,5}^-$ $\Rightarrow \delta_L = -1$

$$(-1)^\nu = (\delta_\Gamma)^1 (\delta_X)^3 (\delta_L)^4 \;\Rightarrow\; \nu = 1$$

- topological insulator

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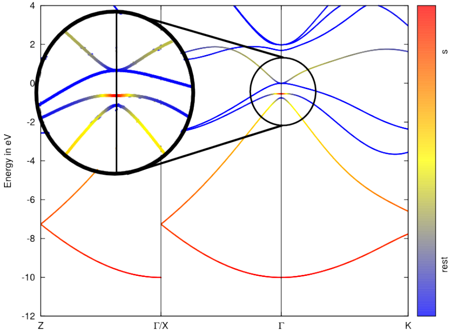

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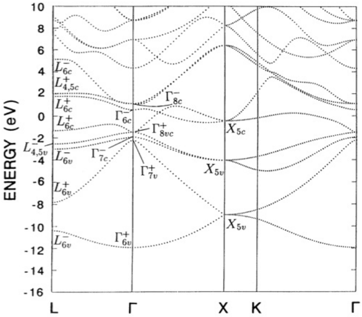

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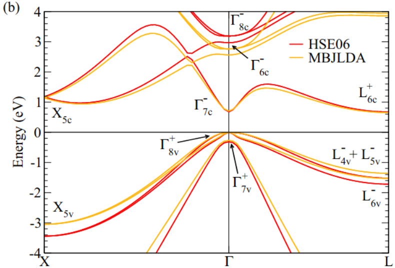

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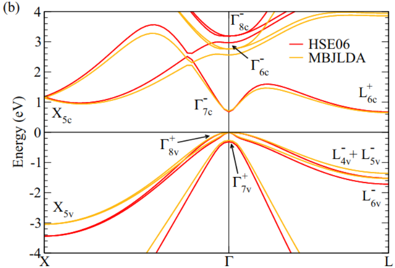
$$(-1)^\nu = (\delta_\Gamma)^1(\delta_X)^3(\delta_L)^4 \;\Rightarrow\; \nu = 0$$

- normal insulator

[4] Rödl *et al.*, PRM **3**, 034602 (2019)

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- Ge (diamond structure)[4], consider lowest two occupied bands - isolated



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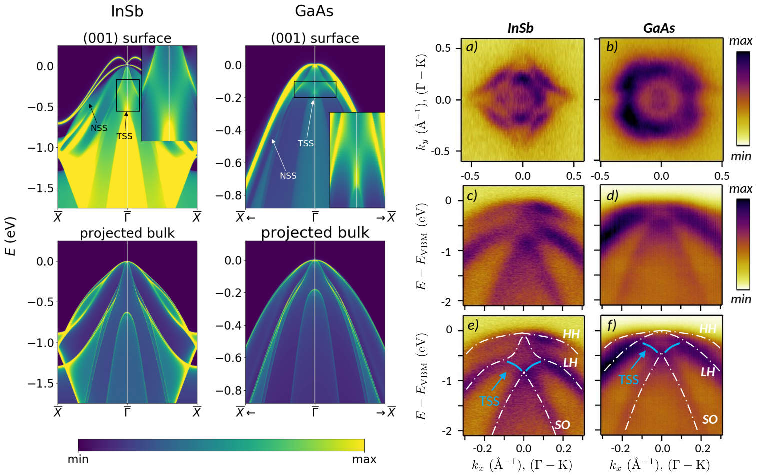
- topological "insulator" (more precisely: group of isolated bands)

[4] Rödl *et al.*, PRM **3**, 034602 (2019)

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- InSb and GaAs aequivalent to Ge[4]:



[4]Rauch *et al.*, PRM **3**, 064203 (2019)

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- in general (e.g. with broken inversion):
  evaluation from wavefunctions in the BZ . . . arbitrary phases
- Berry connection (and other quantities) not gauge-invariant:

$$|u_n(\boldsymbol{k})\rangle \to e^{i\beta(\boldsymbol{k})}|u_n(\boldsymbol{k})\rangle \quad \Rightarrow \quad \boldsymbol{A}_n(\boldsymbol{k}) \to \boldsymbol{A}_n(\boldsymbol{k}) + \nabla_{\boldsymbol{k}}\beta(\boldsymbol{k})$$

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- solution: discretized Berry phase on equividistant mesh: $\{k_j : j = 0, N\}$ with $|u_n(k_N)\rangle = |u_n(k_0)\rangle$

$$\begin{aligned}\gamma_n &= -\Im \ln \prod_{j=0}^{N-1} \langle u_n(k_j)|u_n(k_{j+1})\rangle \\ &= -\Im \ln \left[\langle u_n(k_0)|u_n(k_1)\rangle\langle u_n(k_1)|u_n(k_2)\rangle \ldots \right. \\ &\quad \left. \ldots \langle u_n(k_{N-2})|u_n(k_{N-1})\rangle\langle u_n(k_{N-1})|u_n(k_0)\rangle\right]\end{aligned}$$

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- multiband formulation: set of J bands isolated from other bands
  - each band isolated: $U(1)$ gauge transformation for each band:
    $|\tilde{u}_{n\boldsymbol{k}} >= e^{-i\beta_n(\boldsymbol{k})}|u_{n\boldsymbol{k}} >$, $\boldsymbol{A}_n(\boldsymbol{k}) = i < u_{n\boldsymbol{k}}|\nabla_{\boldsymbol{k}} u_{n\boldsymbol{k}} >$
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  - J bands with degeneracies: $U(J)$ gauge transformation:
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$$\gamma = \oint d\boldsymbol{k}\, \mathrm{Tr}\left[\boldsymbol{A}(\boldsymbol{k})\right] = -\Im \ln \det \prod_{j=0}^{N-1} M^{(k_j, k_{j+1})}$$

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  - sum of phases of eigenvalues of $\prod_{j=0}^{N-1} M^{(k_j,k_{j+1})}$

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- *ab-initio* calculation - above procedure in principle directly applicable

[5] Rauch *et al.*, PRL **114**, 236805 (2015)
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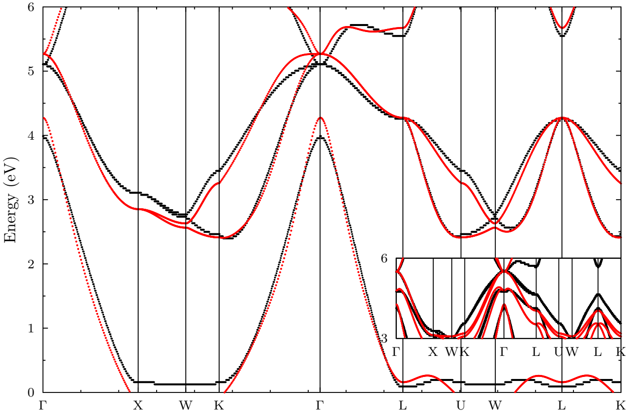

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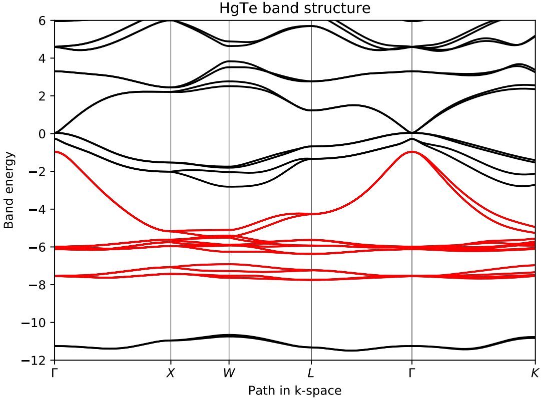

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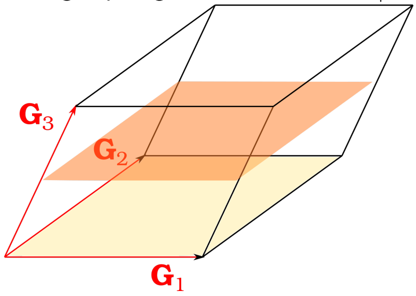

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- for each TRI plane: evolution of hybrid polarization $P_1^h(k_2)$
  e.g. with PythTB
  (http://www.physics.rutgers.edu/pythtb/index.html)
  or Z2Pack[6]

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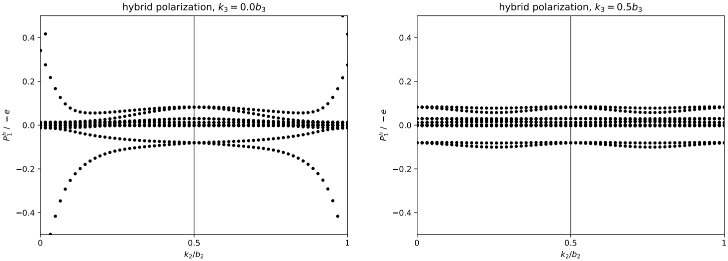
Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

```
# TB matrix H(k) known, stored in my_model

Nx = 21 # k-mesh for hybrid polarization P_1
Ny = 63 # k-mesh along k_2
k_z = 0.5 #nu_2 or \tilde{nu}_2

# array for wave functions
wf = wf_array(my_model,[Nx,Ny])

# prepare the k-mesh (in units of reciprocal lattice vectors)
kpts = []
for i in range(Nx):
    for j in range(Ny):
        kpt = [float(i)/Nx,float(j)/Ny,k_z]
        kpts.append(kpt)

# solve the TB matrix on the k-mesh
eval,evec = my_model.solve_all(kpts,eig_vectors = True)

# copy the wave functions on the array wf
ivec = 0
for i in range(Nx):
    for j in range(Ny):
        wf[i,j] = evec[:,ivec]
        ivec += 1

# impose PBCs
wf.impose_pbc(mesh_dir = 0, k_dir = 0)

# calculate the individual hybrid polarizations P_1 for each k2 on the mesh
wan_cent = wf.berry_phase([2,3,4,5,6,7,8,9,10,11,12,13],dir=0,contin=False,berry_evals=True)
wan_cent/=(2.0*np.pi)

# plot
nky=wan_cent.shape[0]
ky=np.linspace(0.,1.,nky)
for i in range(12):
    ax.plot(ky,wan_cent[:,i],"k.")
```

Practical calculation of the $\mathcal{Z}_2$ topological invariant (3D)

- result for chosen 12 bands of HgTe:



- $\nu_0 = |1 - 0| = 1 \rightarrow$ topologically non-trivial set of bands

Conclusion

- calculation of topological invariants ($\mathcal{Z}_2$ or Chern number)
- next (possibilities):
  - more theoretical concepts
    - (hybrid) Wannier functions
    - other topological classes (TIs protected by other symmetries)
    - magnetoelectric coupling
  - more "practical" information
    - role of spin-orbit coupling
    - properties of surface states of TIs
    - experiments (transport, ARPES, STM)