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
- TBA 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

Berryology[1]

- Berry phase for a closed loop $C = \partial S$

$$\begin{aligned}\gamma_n &= \int_C \boldsymbol{A}_n(\boldsymbol{R}) \cdot d\boldsymbol{R} \\ &= \iint \boldsymbol{\Omega}_n(\boldsymbol{R}) \cdot d\boldsymbol{S}\end{aligned}$$

- Berry connection

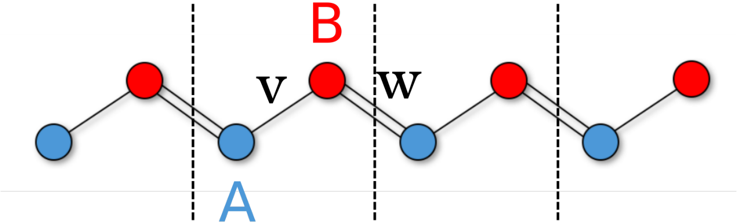
$$\boldsymbol{A}_n(\boldsymbol{R}) = i \left\langle n\left(\boldsymbol{R}\right) \left|\nabla_R\right| n\left(\boldsymbol{R}\right)\right\rangle$$

- Berry curvature

$$\begin{aligned}\boldsymbol{\Omega}_n(\boldsymbol{R}) &= \nabla_R \times \boldsymbol{A}_n(\boldsymbol{R}) \\ &= i \left\langle \nabla_R n\left(\boldsymbol{R}\right) \right| \times \left| \nabla_R n\left(\boldsymbol{R}\right)\right\rangle \\ &= i \sum_{m \neq n} \frac{\left\langle n\left(\boldsymbol{R}\right) \left|\nabla_R H(\boldsymbol{R})\right| m\left(\boldsymbol{R}\right)\right\rangle \times \left\langle m\left(\boldsymbol{R}\right) \left|\nabla_R H(\boldsymbol{R})\right| n\left(\boldsymbol{R}\right)\right\rangle}{\left(E_m(\boldsymbol{R}) - E_n(\boldsymbol{R})^2\right)}\end{aligned}$$

[1] M. Berry, Proc. R. Soc. Lond. A **392**, 45 (1984)

1D example: SSH model[2]



tight-binding Hamiltonian:

$$H(k) = \begin{pmatrix} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{pmatrix} = d_x(k)\sigma_x + d_y(k)\sigma_y$$

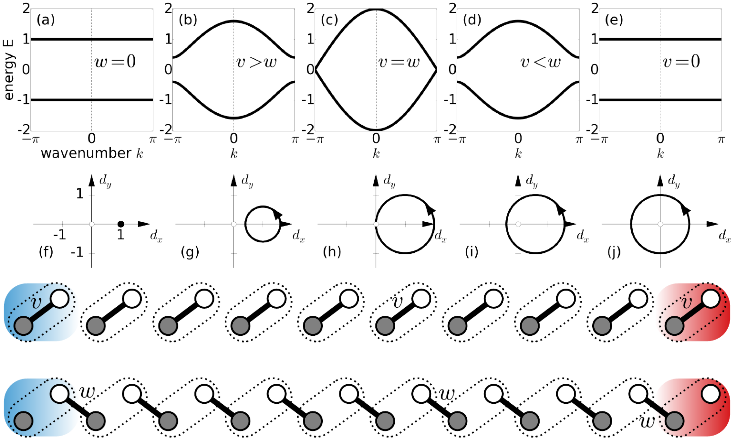
with:

$d_x(k) = v + w\cos(k)$
$d_y(k) = w\sin(k)$
$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

[2] Armitage and Wu, SciPost Phys. **6**, 046 (2019)

1D example: SSH model[3]

$$E_{\pm}(k) = \pm\sqrt{v^2 + w^2 + 2vw\cos(k)}$$



[3]Short course on topological insulators, arXiv:1509.02295

1D example: SSH model

Berry phase of the SSH model:

$$\frac{2\pi P}{-e} = \gamma = \int_{-\pi}^{\pi} dk\ A(k) = \frac{\pi}{2}\left[1 + \operatorname{sgn}\left(\frac{v-w}{v+w}\right)\right]$$

- $v > w$: $P = 0$ and $Q_{\mathrm{surf}} = 0$ ... trivial
- $v < w$: $P = e/2$ and $Q_{\mathrm{surf}} = e/2$ ... non-trivial

Adiabatic transport

towards 2D topological insulators

- assume $P = P\left(\lambda\left(t\right)\right)$

$$\Delta P = P(\lambda_f) - P(\lambda_i) \mod e$$

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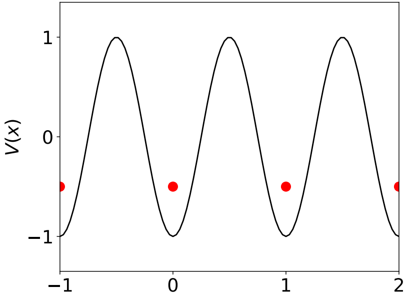
- periodic evolution: $\lambda(0) = \lambda(2\pi)$

$$\Delta P = \begin{cases} 0 & \text{trivial} \\ Ne & \text{non-trivial} \end{cases}$$

Adiabatic transport

$$V(x,\lambda) = -(1 + 0.3\sin(\lambda))\cos(2\pi x)$$



$\lambda = 0$

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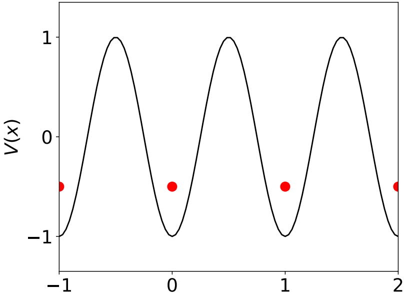

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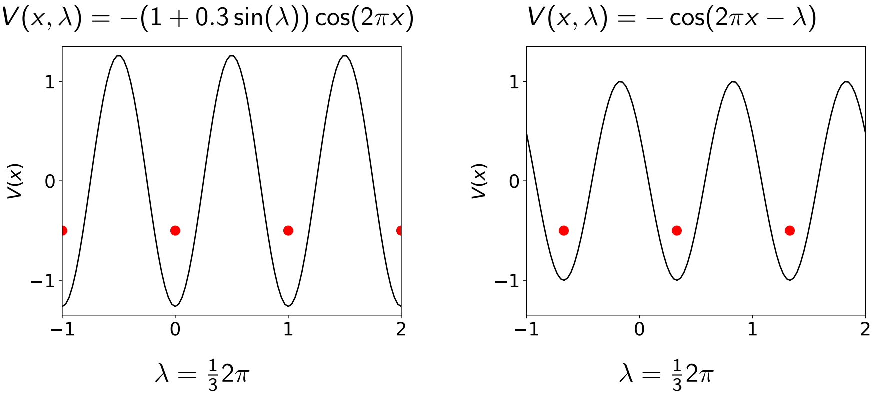

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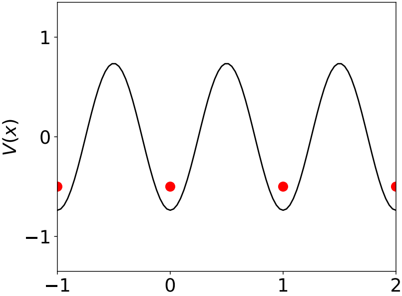

$$\lambda = \frac{2}{3}2\pi$$

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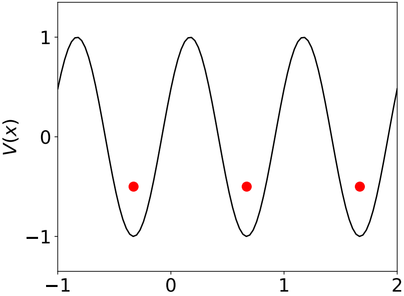

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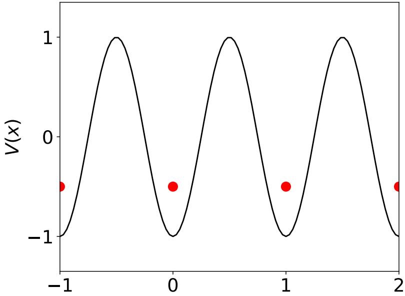

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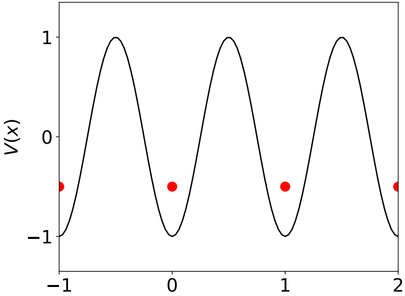

$$\lambda = 2\pi$$

Charge transported between neighboring unit cells during one cycle:

$Q = 0$ $\qquad\qquad$ $Q = e$

Adiabatic transport

2D insulator in electric field E_x, concentrate on change of P_y

- adiabatic parameters (k_x, k_y)
- semiclassical EOM:

$$\frac{dk_x}{dt} = -\frac{e}{\hbar} E_x$$

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- current density pumped along y during one period Δt:

$$j_y = \frac{I_y}{a} = \frac{1}{a}\frac{\Delta P_y}{\Delta t} = \frac{1}{a}\frac{Ne}{\left(-\frac{h}{eaE_x}\right)} = -N\frac{e^2}{h}E_x$$

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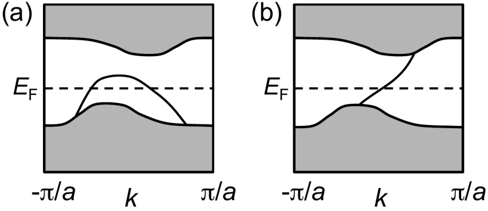
- Hall conductivity:

$$\sigma_{yx} = -N\frac{e^2}{h} \quad \ldots \text{ quantized}$$

Edge states

Edge band structure of a 2D insulator, broken T



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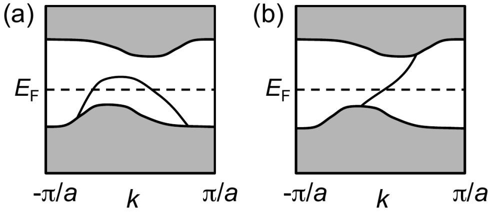

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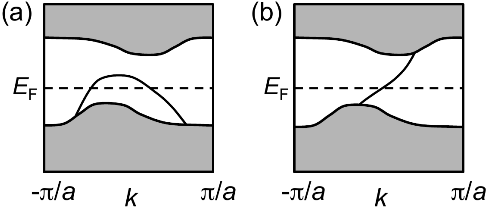

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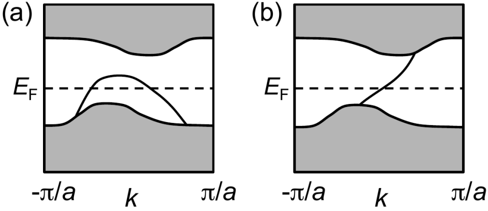

- states at E_F contribute to edge current I_x
- How does I_x vary with change of E_F? $E_F : E_1 \to E_2$
- one state (b) with $v_g = \frac{1}{\hbar}\frac{dE}{dk}$:

$$\Delta I_x = \int_{k_1}^{k_2} \frac{dk}{2\pi}(-e)v_g = -\frac{e}{2\pi\hbar}\int_{k_1}^{k_2}\frac{dE}{dk} = -\frac{e}{h}(E_2 - E_1)$$

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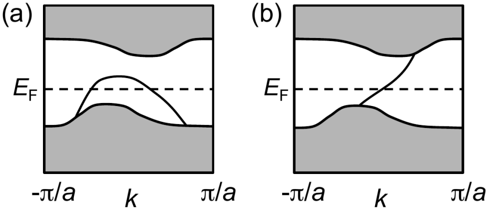

- change of I_x with applied potential ϕ (rigid bands shift):

$$\frac{\partial I_x}{\partial \phi} = e\frac{\partial I_x}{\partial E_F} = -\frac{e^2}{h} \quad \ldots \text{ conductance } G$$

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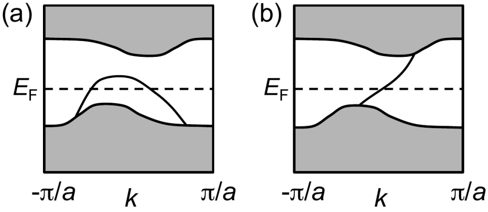

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- multiple edge states:

$$G = (n_{\mathrm{right}} - n_{\mathrm{left}})\frac{e^2}{h} = N\frac{e^2}{h}$$

2D insulators

- bulk: N - change in polarization (Chern number)

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

- edge: N - number of edge states

$$G = N\frac{e^2}{h}$$

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- bulk-boundary correspondence

Topological classification of 2D insulators with broken time-reversal (TR) symmetry

- topological invariant:
  - change in polarization: $\Delta P_y(\Delta k_x : 0 \to 2\pi/a) = -eN$
  - Chern number: $N = \frac{1}{2\pi} \sum_n^{\mathrm{occ}} \int_{\mathrm{BZ}} d^2k \; \Omega_z^n$
    - TR preserved: $N = 0$
    - TR+I preserved: $\Omega_z^n = 0$
  - anomalous Hall conductivity: $\sigma_{xy} = N \frac{e^2}{h}$

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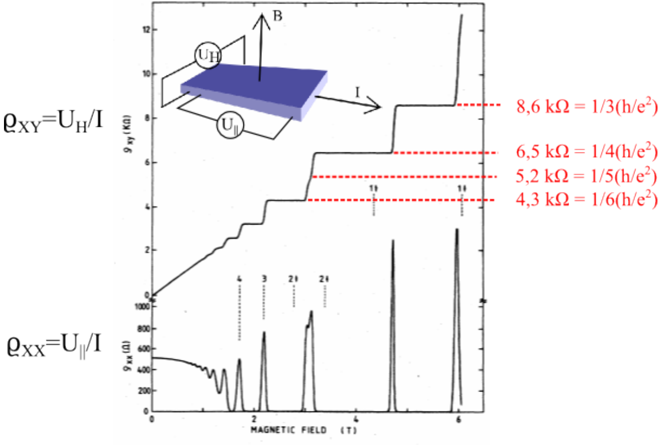
- Do systems with $N \neq 0$ actually exist?

Topological classification of 2D insulators with broken time-reversal (TR) symmetry

- 1980: quantum Hall effect, PRL **45** 494 (1980)
  - experimental realization with external magnetic field



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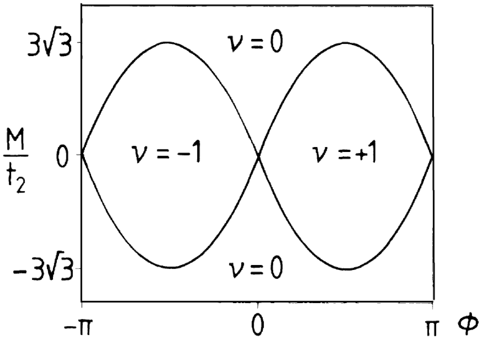

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- 2013: quantum anomalous Hall effect, Science **340** 167 (2013)
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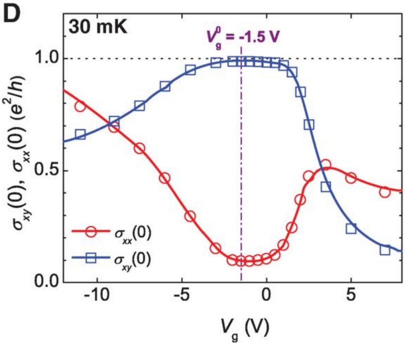

2D insulators with time-reversal (TR) symmetry

role of TR operator θ with $\theta^2 = -1$:

- eff. Hamiltonian: $\theta^{-1} H(\boldsymbol{k}) \theta = H(-\boldsymbol{k})$
- band structure: $E_n^I(\boldsymbol{k}) = E_n^{II}(-\boldsymbol{k})$
- wave functions: $\left|u_n^I(-\boldsymbol{k})\right\rangle = \theta \left|u_n^{II}(\boldsymbol{k})\right\rangle$, $\left|u_n^{II}(-\boldsymbol{k})\right\rangle = -\theta \left|u_n^I(\boldsymbol{k})\right\rangle$
- 1D polarization: $P_y^I(\boldsymbol{k}) = P_y^{II}(-\boldsymbol{k})$

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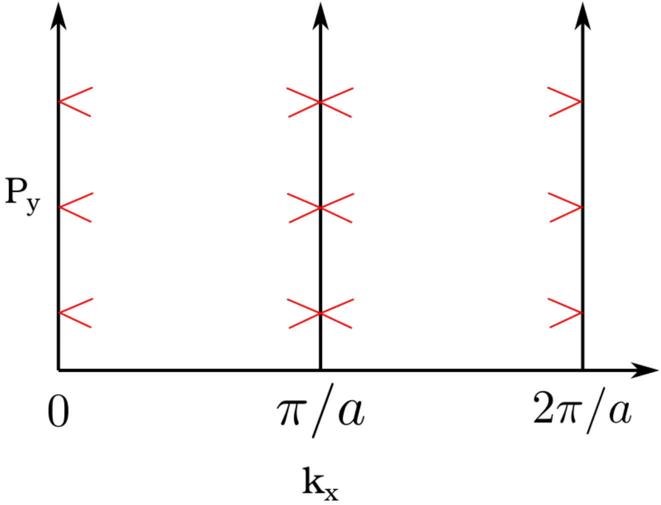
at time-reversal invariant momenta (TRIMs):

- TRIMs: $\boldsymbol{k} = -\boldsymbol{k} + \boldsymbol{G}$
- $P_y^I(k_i) = P_y^{II}(k_i)$ at $k_i = \{0, \pm\pi/a\}$

2D insulators with time-reversal (TR) symmetry

connectivity of $P_y^{I/II}(k_x)$ curves:



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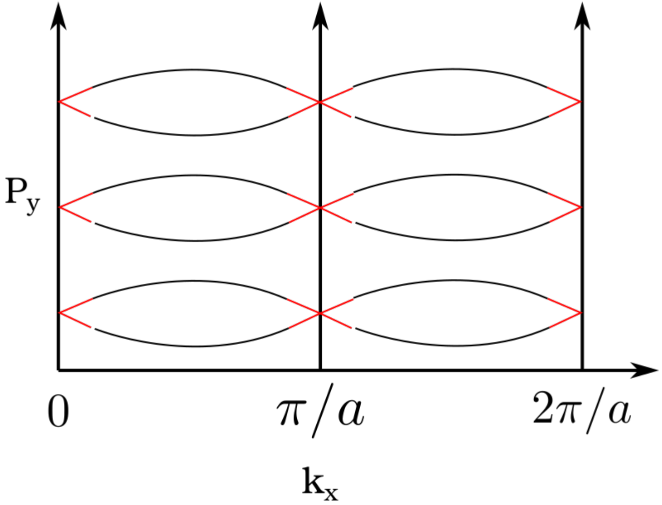

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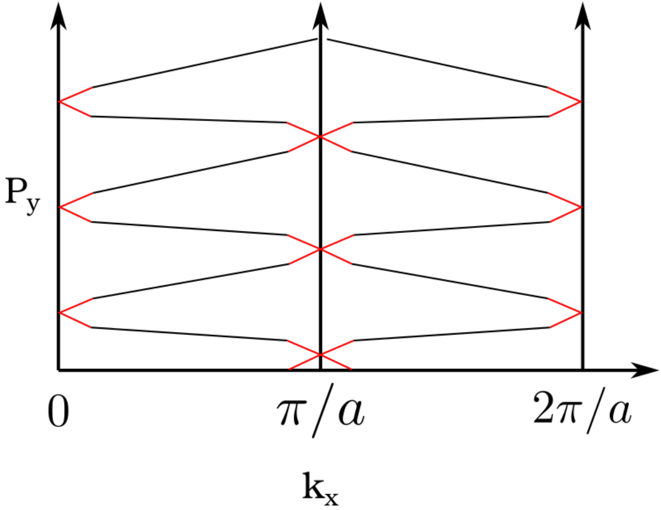

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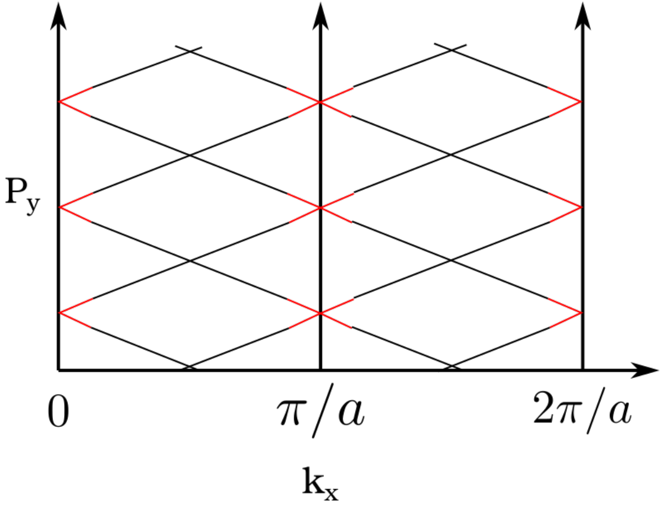
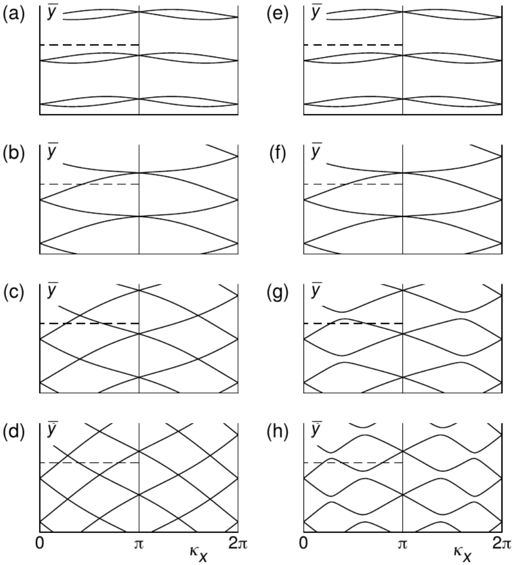


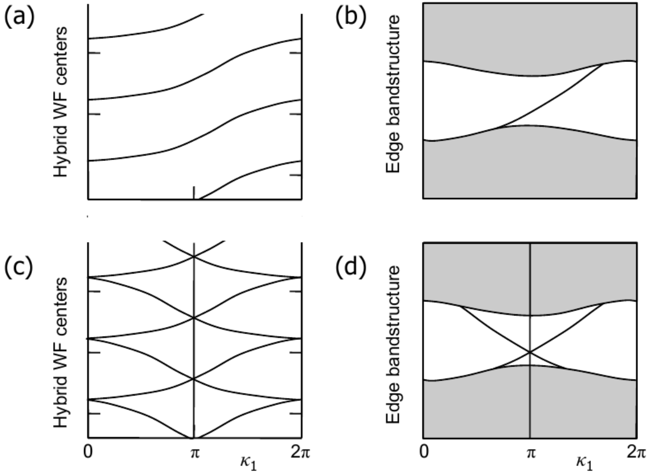
2D insulators with time-reversal (TR) symmetry

number N_c of crossings with a reference line $P_y = c$: $\nu = N_c \mod 2$



2D insulators with time-reversal (TR) symmetry

flow of polarization $\leftrightarrow$ edge-state dispersion



Topological classification of TR-symmetric 2D insulators[4]

- topological invariant:
  - connectivity of $P_y(\Delta k_x : 0 \to 2\pi/a)$: $\nu = N_c \mod 2$
  - $\nu = 0$: trivial, $\nu = 1$: nontrivial("topological")
  - can be calculated also by other means

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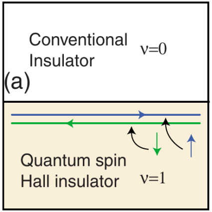
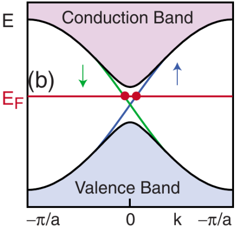
- ν pairs of edge states bridging the band gap:
  - right-going channel: velocity v, charge e, spin s
  - left-going channel: velocity $-v$, charge e, spin $-s$
  - edge charge current: $I = ev + e(-v) = 0$
  - edge spin current: $I^s = sv + (-s)(-v) = 2sv$





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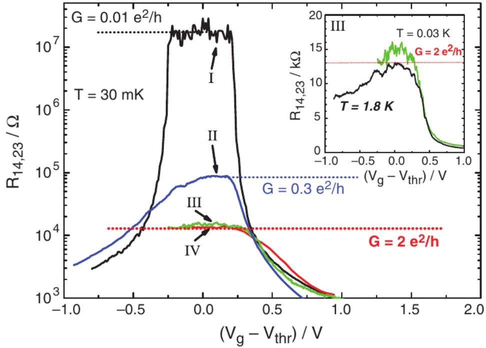
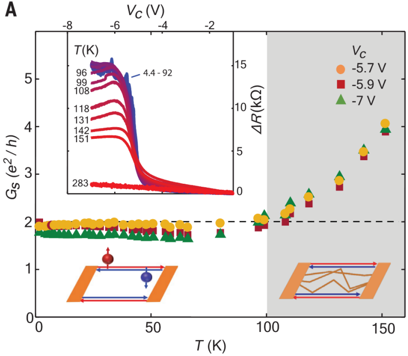
- 2007: HgCdTe quantum wells: König *etal.*, Science **318**, 766 (2007)
  - first experimental realization



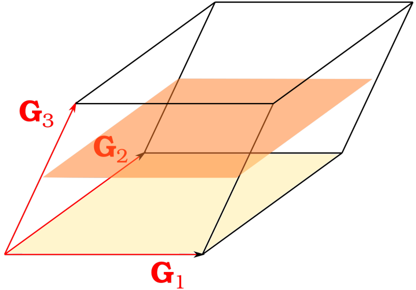
Topological classification of TR-symmetric 2D insulators

- 2005: theoretical predictions: Kane, Mele, PRL **95**, 146802 (2005)
- 2007: HgCdTe quantum wells: König *etal.*, Science **318**, 766 (2007)
  - first experimental realization
- 2018: WTe_2: Wu *et al.*, Science **359**, 76 (2018)
  - more recent experiments



3D insulators with TR symmetry

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



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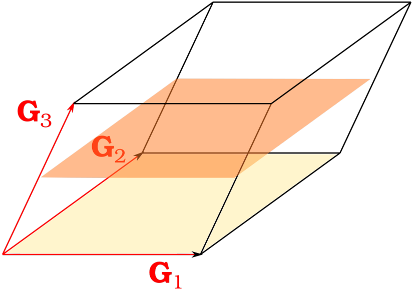

- torus geometry: six topological $\mathbb{Z}_2$ invariants protected by TR

3D insulators with TR symmetry

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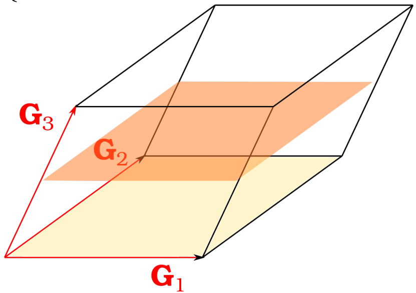

- torus geometry: six topological $\mathbb{Z}_2$ invariants protected by TR
- only four independent invariants: $(\nu_0; \nu_1\nu_2\nu_3)$
  - $(0; 000)$ trivial insulator
  - $(0; \nu_1\nu_2\nu_3)$ weak topological insulator ... stacked 2D TIs
  - $(1; \nu_1\nu_2\nu_3)$ strong topological insulators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