Introduction to topology in electronic structure of crystalline solids

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IFTO, FSU Jena

Schedule

- 24.03. Introduction into topological insulators
- 14.04. 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

for theoretical discoveries of topological phase transitions and topological phases of matter

Fig. from nobelprize.org

Topology in mathematics

[1] H. Eschrig: Topology and Geometry for Physics, Springer (2011)
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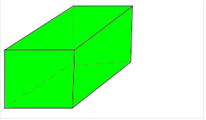

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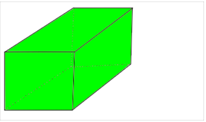

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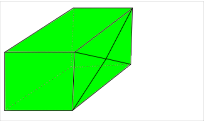

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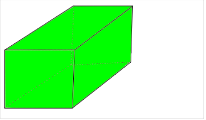

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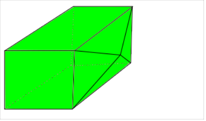

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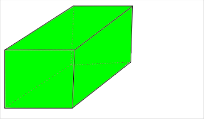

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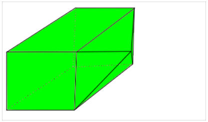

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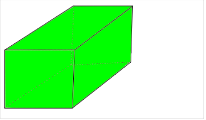

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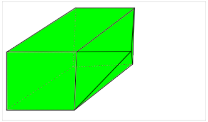

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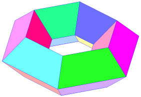

$$\chi = 24 - 48 + 24 = 0$$

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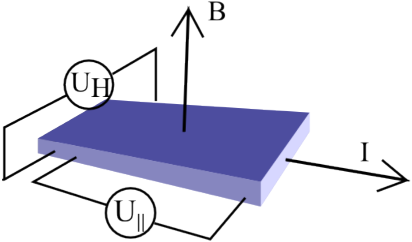
Topology in solid-state physics (example)[2]

Quantum Hall effect



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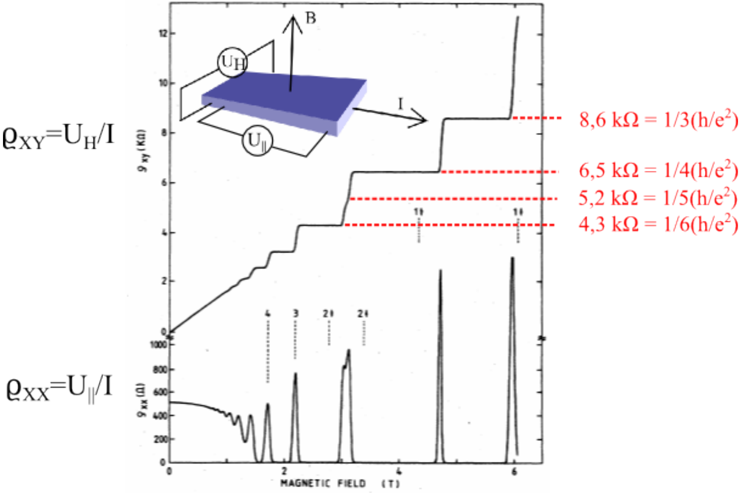

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Berryology[3]

- time-varying Hamiltonian $H(\boldsymbol{R})$ with parameters $R_i = R_i(t)$

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- How will the phase $\theta(t)$ of $|\psi(t)\rangle = e^{-i\theta(t)}\,|n(\boldsymbol{R}(t))\rangle$ evolve?
- Given by

$$H(\boldsymbol{R}(t))\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle$$

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Berryology[4]

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

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

- Berry connection

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

- Berry curvature

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

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    $\Rightarrow$ Berry phase of electrons in solids:

$$\varphi_n(C) = i \int_C \langle u_n(\boldsymbol{k}) | \nabla_{\boldsymbol{k}} u_n(\boldsymbol{k}) \rangle \cdot d\boldsymbol{k}$$

Example: polarization in 1D[5]

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

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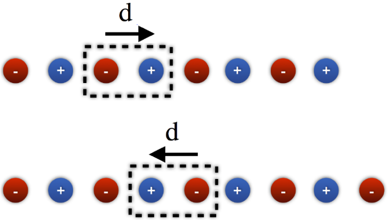

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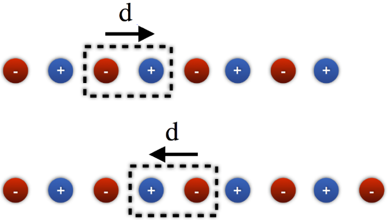

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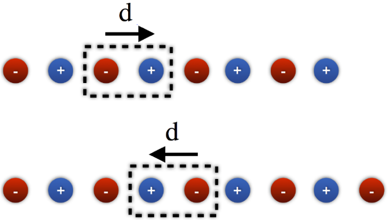

  - Modern theory:

$$P = -\frac{e}{2\pi}\sum_{n}^{\text{occ}}\gamma_n = -\frac{e}{2\pi}\sum_{n}^{\text{occ}}\int_0^{2\pi/a} A_n(k)dk$$

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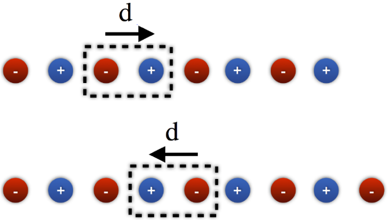

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    - defined only modulo e ... Berry connection not gauge invariant

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- macroscopic charge density $\rho(x) = -\frac{d}{dx}P(x)$
  - surface charge:

$$\begin{aligned} Q_{\mathrm{surf}} &= \int_{\mathrm{bulk}}^{\mathrm{vac}} dx \rho(x) \\ &= -\int_{\mathrm{bulk}}^{\mathrm{vac}} dx \frac{d}{dx} P(x) \\ &= -(P_{\mathrm{vac}} - P_{\mathrm{mat}}) \mod e = P_{\mathrm{mat}} + ne \\ &= ne + \begin{cases} 0 & \text{trivial} \\ e/2 & \text{non-trivial} \end{cases} \end{aligned}$$

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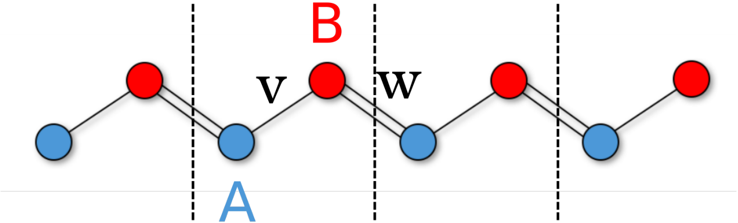
  - phase transition only via breaking of the adiabatic assumption $\leftrightarrow$ closing of the band gap
  - (mostly) presence of boundary states in the band gap

1D example: SSH model[6]



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:

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

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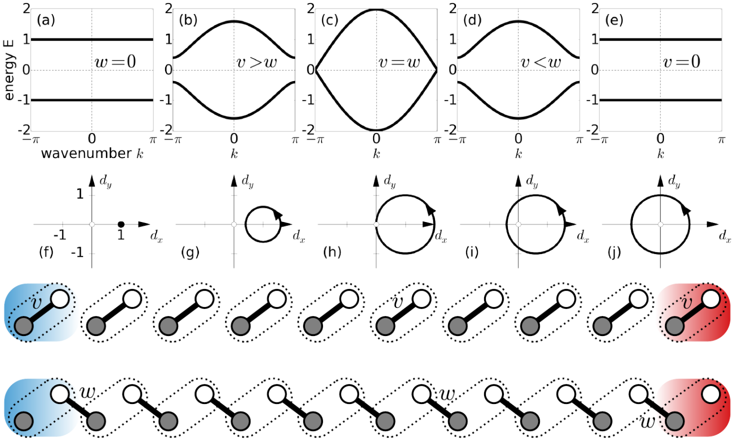
1D example: SSH model[7]

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



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

1D example: SSH model

Berry phase of the SSH model:

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

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

Adiabatic transport

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

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

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

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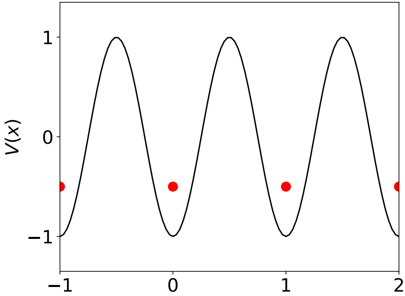
$V(x, \lambda) = -(1 + 0.3 \sin(\lambda)) \cos(2\pi x)$



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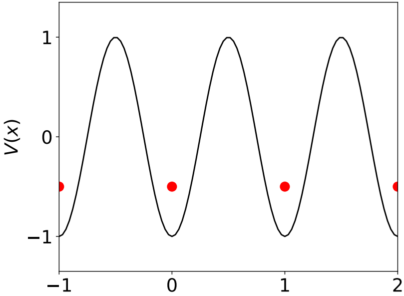

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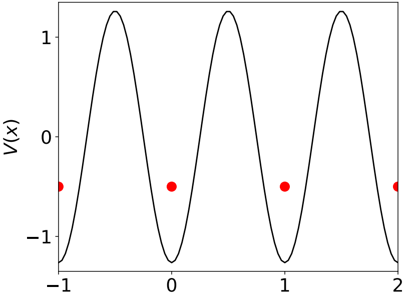

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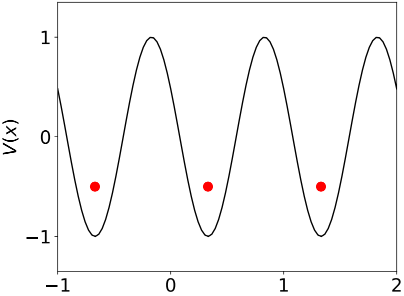

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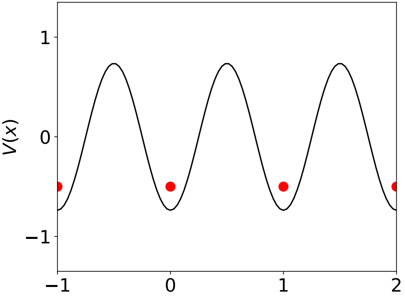

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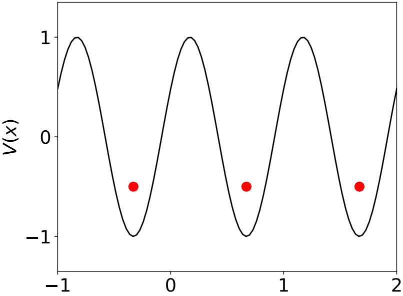

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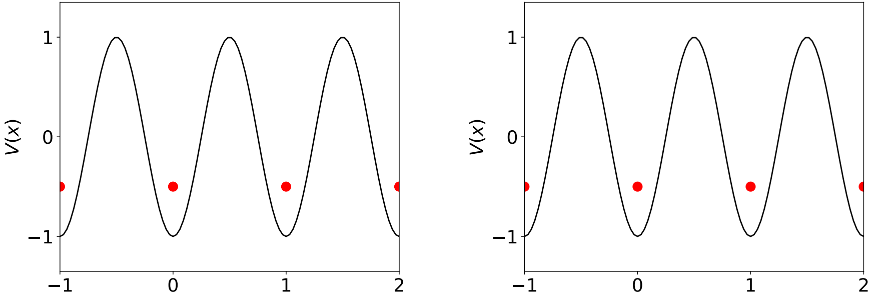

$\lambda = 2\pi$ $\qquad$ $\lambda = 2\pi$

Charge transported between neighboring unit cells during one cycle:

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