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. Role of spin-orbit coupling, band inversions and experimental evidence
- 05.05. (Hybrid) Wannier functions
- 12.05. Higher-order topological insulators, topological metals, skyrmions, Majorana fermions
- 19.05. Applications, conclusions, open questions

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

Conclusion

- basic concepts: adiabatic evolution of wave function
- basic quantities: “Berryology”
- topological insulators in 1D, 2D, 3D
- relation to surface states
- spin-orbit coupling, band inversions, experiments
- hybrid Wannier function - alternative to Bloch functions
- recent research: HOTIs, topological metals

Ideal properties of topological insulators[1]

[1] Tian *et al.*, Materials **10**, 814 (2017)

Ideal properties of topological insulators[1]

- insulating bulk
  - low resistivity

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Ideal properties of topological insulators[1]

- insulating bulk
  - low resistivity
- metallic surface states
  - "robust" against deformations
  - linear dispersion relation
    $\rightarrow$ high mobility (c.f. graphene)
  - low dissipation (elastic backscattering at impurities forbidden)
    $\rightarrow$ low power consumption of TI-based devices, low heat production
  - spin-polarized
    $\rightarrow$ electron spin as information / signal, interaction with magnetic materials: spintronics

[1] Tian *et al.*, Materials **10**, 814 (2017)

Problems

- bulk often not insulating due to defects
- band gap typically limited by SOC strength
- linear dispersion of surface states only close to the Dirac point
- non-elastic scattering allowed: finite mean-free path
- additional surface states can spoil the properties

Some envisioned applications

- topological quantum computing through Majorana fermions
- low-dissipation electronics (via surface/edge states)
- spintronics (via electron spin of the surface/edge state)

Some more concrete examples

Surface-state enhanced photothermoelectric effect in Bi_2Se_3[2]

- circular-polarized light
- surface electrons with a given spin orientation excited
- spin orientation related to momentum
- enhancement of oriented electron transport in temperature gradient (Bi_2Se_3 good thermoelectric material)
- use as photodetector?

[2] Yan *et al.*, Nano Lett. **14**, 4389 (2014)

Some more concrete examples

Field-effect transistor[3]

- switching topological↔trivial: too large electric field necessary
- on/off state characterized by the strength of backscattering controlled by gate voltage (theory)
- more on “Topological electronics”[4]
(not to mix with “Topoelectrics”)

[3] Vandenberghe *et al.*, Nature Communications **8**, 14184 (2017)
[4] Gilbert, Communications Physics **4**, 70 (2021)

Some more concrete examples

Intrinsically core-shell plasmonic dielectric nanostructures with ultrahigh refractive index[5]

- plasmonic metallic nanostructures useful in optical devices
- but: large loss in visible frequency range
- dielectric nanostructures can bridge the problem
- but: nanostructuring complicated on a larger scale
- TI: natural dielectric with metallic surface

[5] Yue *et al.*, Science Advances **2**, e1501536 (2016)

Some more concrete examples

Nanometric holograms based on a topological insulator material[6]

- phase shift necessary, thickness limited in conventional materials
- TI: insulating bulk + metallic surface → intrinsic resonant cavity
- very thin holograms possible

[6] Yue *et al.*, Nature Communications **8**, 15354 (2017)

Transfer of topological classification to other systems

- key quantity can be mapped to electronic Hamiltonian
- topological classification possible
- guaranteed surface/edge modes

[7] Wang *et al.*, Journal of Applied Physics **129**, 151101 (2021)
[8] Liu *et al.*, Adv. Funct. Mater. **30**, 1904784 (2020)
[9] Ozawa *et al.*, Rev. Mod. Phys. **91**, 015006 (2019)
[10] Lee *et al.*, Communications Physics **1**, 39 (2018)

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- **magnon** Hamiltonian[7]

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- **admittance matrix** of electrical circuits[10] (Topoelectrics)

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Remaining questions?