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
- 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

Wannier functions

- assume isolated band $E_{n\mathbf{k}}$
  - smooth and periodic in reciprocal space
  - Fourier-transform to real space:

$$E_{n\mathbf{R}} = \frac{V_{\mathrm{cell}}}{(2\pi)^3} \int_{\mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}} E_{n\mathbf{k}} \, d^3k$$

$$E_{n\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} E_{n\mathbf{R}}$$

  - $E_{n\mathbf{R}}$ expected to decay rapidly with increasing $|\mathbf{R}|$

Wannier functions

- assume smooth and periodic gauge for $|\psi_{n\mathbf{k}}\rangle$

$$|w_{n\mathbf{R}}\rangle = \frac{V_{\mathrm{cell}}}{(2\pi)^3} \int_{\mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n\mathbf{k}}\rangle \; d^3k$$

$$|\psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |w_{n\mathbf{R}}\rangle$$

- $|w_{n\mathbf{R}}\rangle$ ...Wannier functions
- unitary transformation of the Bloch state $|\psi_{n\mathbf{k}}\rangle$
  - $|\psi_{n\mathbf{k}}\rangle$ and $|w_{n\mathbf{R}}\rangle$ describe the same manifold of states

Wannier functions

Properties:

Wannier functions

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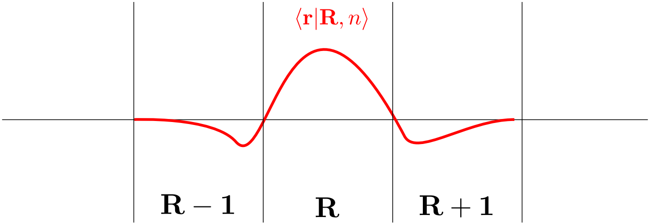
1. $|w_{n\mathbf{R}}\rangle$ localized in real space: $|w_{n\mathbf{R}}(\mathbf{r})| \to 0$ for large $|\mathbf{r} - \mathbf{R}|$



Wannier functions

Properties:

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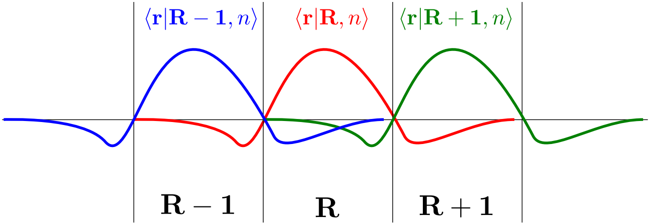

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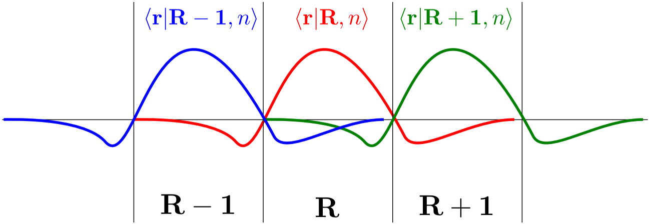

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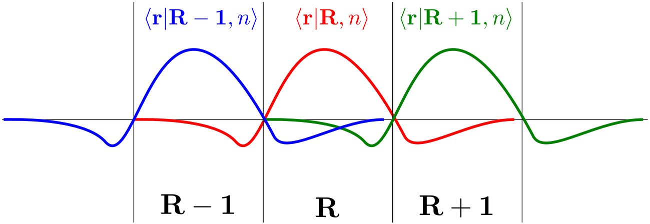
3. orthonormal: $\langle w_{n\mathbf{R}}|w_{n\mathbf{R}'}\rangle = \delta_{\mathbf{R}\mathbf{R}'}$
4. span the same subspace of the Hilbert space as $\{|\psi_{n\mathbf{k}}\rangle\}$:
   - projection operator: $P_n = \frac{V_{\mathrm{cell}}}{(2\pi)^3}\int_{\mathrm{BZ}} |\psi_{n\mathbf{k}}\rangle\langle\psi_{n\mathbf{k}}|\ d^3k = \sum_{\mathbf{R}} |w_{n\mathbf{R}}\rangle\langle w_{n\mathbf{R}}|$
   - charge density:
     $\rho_n(\mathbf{r}) = -e\langle\mathbf{r}|P|\mathbf{r}\rangle = -e\frac{V_{\mathrm{cell}}}{(2\pi)^3}\int_{\mathrm{BZ}} |\psi_{n\mathbf{k}}(\mathbf{r})|^2 = -e\sum_{\mathbf{R}} |w_{n\mathbf{R}}(\mathbf{r})|^2$



Wannier functions

Properties:

5. Hamiltonian matrix elements:

$$\langle w_{n\mathbf{0}}|H|w_{n\mathbf{R}}\rangle = E_{n\mathbf{R}}$$

- exact tight-binding representation of $E_{n\mathbf{k}}$
- $E_{n\mathbf{0}}$ ...on-site terms
- $E_{n\mathbf{R}}$ ...hoppings - fast decay with large $|\mathbf{R}|$
- Wannier interpolation (not only for energy bands)

Wannier functions

Properties:

6. position matrix elements:

$$\langle w_{n\mathbf{0}}|\mathbf{r}|w_{n\mathbf{R}}\rangle = \mathbf{A}_{n\mathbf{R}}$$

- Fourier transform of Berry connection

$$\mathbf{A}_{n\mathbf{R}} = \frac{V_{\mathrm{cell}}}{(2\pi)^3}\int_{\mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}}\mathbf{A}_{n\mathbf{k}}\ d^3k$$
$$\mathbf{A}_{n\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\mathbf{A}_{n\mathbf{R}}$$

- Wannier charge centers $\bar{\mathbf{r}}_n = \langle w_{n\mathbf{0}}|\mathbf{r}|w_{n\mathbf{0}}\rangle = \int_{\mathrm{BZ}}\mathbf{A}_{n\mathbf{k}}\ d^3k$
- 1D: $\overline{x}_n = \frac{a}{2\pi}\int_0^{2\pi/a} A_n(k)dk = \frac{a}{2\pi}\phi_n = -\frac{1}{e}Px$
  $\phi_n\ldots$Berry phase, $P_x\ldots$electric polarization
- topological invariants: $P_x(k_y)$ equivalent to $\bar{x}_n(k_y)$

Wannier functions

Gauge transformations
one band: $|u_{\mathbf{k}}\rangle \to e^{-i\beta(\mathbf{k})}|u_{\mathbf{k}}\rangle$

[1] G. Pizzi *et al.*, J. Phys. Cond. Matt. **32**, 165902 (2020)

Wannier functions

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- $E_{n\mathbf{k}}$ and $E_{n\mathbf{R}}$ gauge invariant

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- $\bar{\mathbf{r}}_n$ gauge invariant modulo $\mathbf{R}$ (1D: 2π ambiguity of ϕ)
- $|w_{n\mathbf{R}}\rangle$ not unique - depend on the gauge choice of Bloch functions
  - fast decay: maximally-localized Wannier functions (MLWFs)
  - minimize quadratic spread

$$\Omega = \sum_n \left[\langle w_{n\mathbf{0}}|\mathbf{r}^2|w_{n\mathbf{0}}\rangle - \bar{\mathbf{r}}^2\right]$$
$$= \Omega_I + \underbrace{\widetilde{\Omega}}_{\text{gauge}-\text{dependent}}$$

  - e.g. with `wannier90`[1]
  - 1D: twisted parallel-transport gauge yields MLWFs

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Wannier functions

Parallel transport:
general (differential geometry, fiber bundles, etc.)

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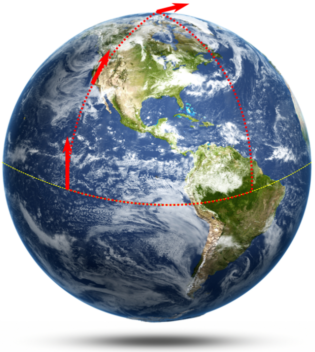

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Parallel transport:
for periodic Bloch-states

- base space: all Hamiltonians $H(\mathbf{k})$ in the BZ
- fiber: at each $\mathbf{k}$: all wavefunctions $e^{-i\beta(\mathbf{k})}|u_{\mathbf{k}}\rangle$
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- numerics: N Bloch states $|\tilde{u}_{k_j}\rangle$ with arbitrary phases on equidistant k-mesh $\{\mathbf{k}_j\}$, $j = 1, \ldots, N+1$
- goal: make neighboring states $|u_{k_j}\rangle$ and $|u_{k_{j+1}}\rangle$ as parallel as possible $\Rightarrow \langle u_{k_j}|u_{k_{j+1}}\rangle$ real, positive

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   $\phi = \overline{x}\ldots$WCC (or Berry phase on the closed path)

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6. $|u_{k_j}\rangle$ smooth and periodic $\Rightarrow$ MLWFs obtained by Fourier transform, WCCs already obtained

Wannier functions

generalization to a manifold of J isolated states:

- $U(J)$ gauge transformation:

$$|\widetilde{\psi}_{n,\mathbf{k}}\rangle = \sum_{m=1}^{J} \mathcal{U}_{mn}(\mathbf{k})|\psi_{m,\mathbf{k}}\rangle, \quad \mathcal{U} \text{ unitary}$$

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- J Wannier centers (diagonal elements):

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$$\widetilde{M}_{ln} = \langle u_l | \widetilde{v}_n \rangle = \sum_{m=1}^{J} \langle u_l | v_m \rangle \left(WV^\dagger\right)_{mn} = \sum_{m=1}^{J} M_{lm} \left(WV^\dagger\right)_{mn}$$

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$$\Rightarrow \widetilde{M} = V\Sigma W^\dagger W V^\dagger = V\Sigma V^\dagger \approx \mathbb{1}, \text{ if } s_n \approx 1\ \forall n$$

Hybrid (hermaphrodite) Wannier functions[2]

[2] Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

Hybrid (hermaphrodite) Wannier functions[2]

- localized along one direction, Bloch-like in remaining directions

$$|w_{nR_x}(k_y, k_z)\rangle = \frac{L}{2\pi} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_x e^{-ik_x R_x} |\psi_{n,\mathbf{k}}\rangle$$

  - $L \dots$ lattice parameter along x
  - $R_x = mL, \; m \in \mathbb{Z}$

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$$\overline{x}_n(k_y, k_z) = \langle w_{n0}(k_y, k_z)|\hat{x}|w_{n0}(k_y, k_z)\rangle$$

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$$\overline{x}_n(k_y, k_z) = \langle w_{n0}(k_y, k_z)|\hat{x}|w_{n0}(k_y, k_z)\rangle$$

- for a fixed $\boldsymbol{\kappa} = (k_y, k_z)$ effectively a 1D problem

[2] Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

Hybrid (hermaphrodite) Wannier functions[2]

- localized along one direction, Bloch-like in remaining directions

$$|w_{nR_x}(k_y,k_z)\rangle = \frac{L}{2\pi}\int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_x e^{-ik_xR_x}|\psi_{n,\mathbf{k}}\rangle$$

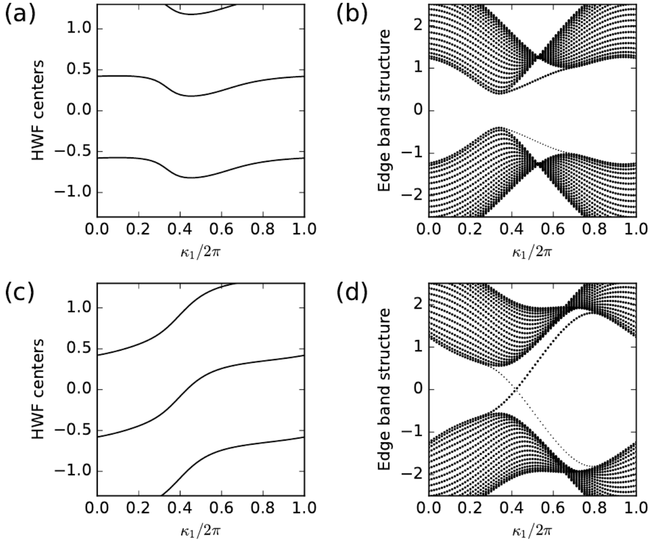
  - $L\ldots$ lattice parameter along x
  - $R_x = mL,\ m \in \mathbb{Z}$
- hybrid WCCs:

$$\overline{x}_n(k_y,k_z) = \langle w_{n0}(k_y,k_z)|\hat{x}|w_{n0}(k_y,k_z)\rangle$$

- for a fixed $\boldsymbol{\kappa} = (k_y,k_z)$ effectively a 1D problem
- remember: topological invariants: $\overline{x}_n(k_y) = -\frac{1}{e}P_x(k_y)$

[2] Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

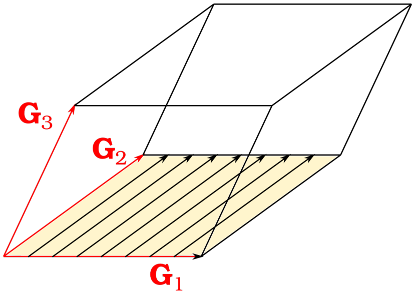
Hybrid (hermaphrodite) Wannier functions[3]



[3]Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

Hybrid (hermaphrodite) Wannier functions[4]

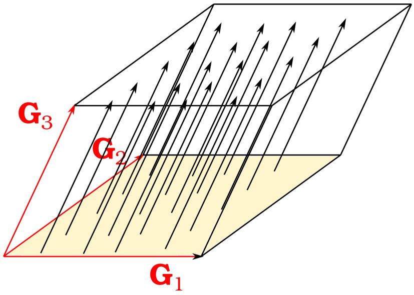
- usually $|u_{n\mathbf{k}}\rangle$ for $\mathbf{k}$ in the plane of interest:
  - 2D materials: $\rightarrow$ $\mathbf{k}$ in 2D BZ
  - 3D materials: $\rightarrow$ $\mathbf{k}$ in 2D time-reversal invariant planes
  - wannierization direction: in the plane of interest



[4]Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

Hybrid (hermaphrodite) Wannier functions[4]

- usually $|u_{n\mathbf{k}}\rangle$ for $\mathbf{k}$ in the plane of interest:
  - 2D materials: $\rightarrow$ $\mathbf{k}$ in 2D BZ
  - 3D materials: $\rightarrow$ $\mathbf{k}$ in 2D time-reversal invariant planes
  - wannierization direction: in the plane of interest
- consider different wannierization direction:
  - hybrid WFs: $|w_{n,R_3}(k_1, k_2)\rangle$
  - hybrid charge centers ($\mathbf{a}_3 \parallel \hat{\mathbf{e}}_z$): $\bar{z}_n(k_1, k_2)$ - Wannier sheets



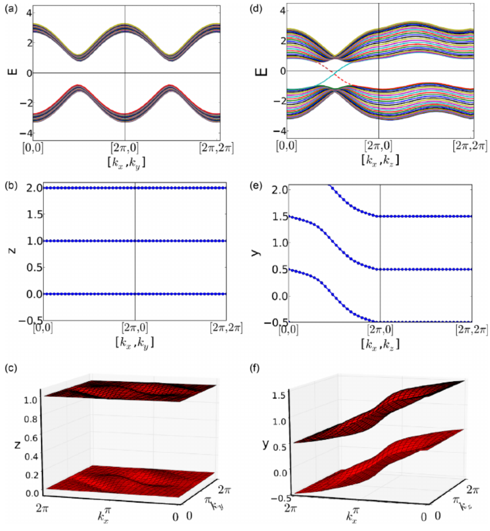
[4] Sgiarovello, Peressi, Resta, PRB **64**, 115202 (2001)

Wannier sheets in topological insulators[5]

[5]Taherinejad *et al.*, PRB **89**, 115102 (2014)

Wannier sheets in topological insulators[5]

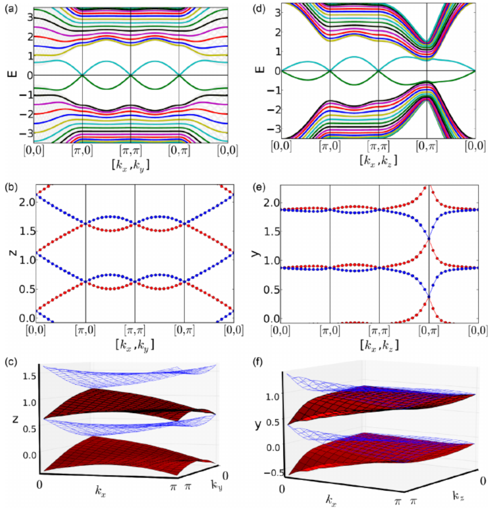
3D stacking of 2D Chern insulator layers



[5] Taherinejad *et al.*, PRB **89**, 115102 (2014)

Wannier sheets in topological insulators[5]

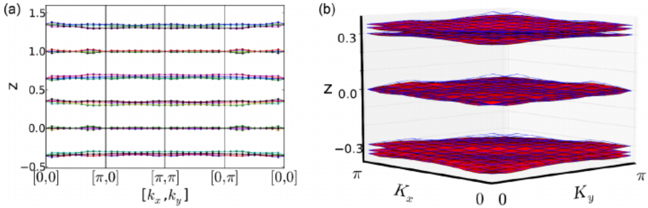
3D strong topological insulator (Fu-Kane-Mele model)



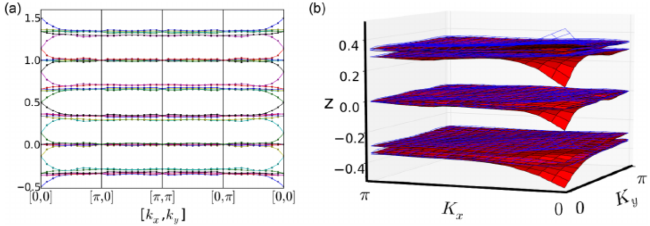
[5] Taherinejad *et al.*, PRB **89**, 115102 (2014)

Wannier sheets in topological insulators[5]

3D normal insulator (Sb_2Se_3 - *ab-initio*)



3D strong topological insulator (Bi_2Se_3 - *ab-initio*)



[5] Taherinejad *et al.*, PRB **89**, 115102 (2014)

Wannier sheets in topological insulators[7]

- Wannier sheets often allow graphical evaluation of topological invariants
- unified approach to some types of topological insulators (e.g. Chern, strong/weak)

[6] Rauch *et al.*, PRB **103**, 195103 (2021)
[7] Taherinejad *et al.*, PRB **89**, 115102 (2014)

Wannier sheets in topological insulators[7]

- Wannier sheets often allow graphical evaluation of topological invariants
- unified approach to some types of topological insulators (e.g. Chern, strong/weak)
- sometimes hybrid Wannier functions are necessary
  - quantities can be defined as for Bloch functions
  - isolated Wannier sheet: Chern number:
    $C_{n,R_z} = \int_{\mathrm{2DBZ}} \Omega_{n,Rz}\ d^2k = C_{n0}$
    Berry curvature: $\Omega_{n,Rz} = -2\mathrm{Im}\,\langle \partial_{k_1} w_{n,Rz} | \partial_{k_2} w_{n,Rz} \rangle$
  - e.g. hybrid Wannier representation of the mirror Chern number[6] (for topological insulators in presence of mirror symmetry)

[6] Rauch *et al.*, PRB **103**, 195103 (2021)
[7] Taherinejad *et al.*, PRB **89**, 115102 (2014)

MLWFs: Wannier interpolation

anomalous Hall conductivity[8]

- BZ integral of the Berry curvature
- also as Kubo-formula: from velocity matrix elements
- in TB: velocity matrix elements / Berry curvature lack contributions from position matrix elements (TB approximation)
- MLWFs: position matrix elements accessible from *ab-initio*
  $\rightarrow$ results should agree exactly with direct *ab-initio* calculation
- applicable to other quantities (e.g., optical conductivity)

[8] Wang *et al.*, PRB **74**, 195118 (2006)

Wannier functions

- general properties
- maximally-localized Wannier functions
- hybrid Wannier functions and charge centers
- relation to topological invariants

Following seminars:

1. topological metals, Weyl-, Dirac-, Majorana-fermions, skyrmions, etc.
2. envisioned applications (discussion?)