Topological insulators and superconductors

Andreas P. Schnyder

Max-Planck-Institut für Festkörperforschung, Stuttgart

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Over the last years, the number of known topological materials has exploded.

Can we bring some order in this zoo of topological materials?
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Classification of chemical elements

Periodic table of the elements

Organize elements according to symmetries of electronic configurations

1860s  Dimitri Mendeleev

prediction of new elements: Ge, Sc, Tc, Ga

Can topological materials be classified in a similar fashion?
Topological insulators and superconductors

1. Topological band theory
   - What is topology?
   - SSH model (polyacetylene)

2. Chern insulators and IQHE
   - Integer quantum Hall effect
   - Chern insulator on square lattice

3. Topological insulators w/ time-reversal symmetry
   - Quantum spin Hall state
   - $\mathbb{Z}_2$ invariants in 2D & 3D

4. Topological superconductors
   - Topological superconductors in 1D & 2D
   - Topological superconductors w/ TRS

5. Classification scheme and topological semi-metals
   - Tenfold classification of TIs and SCs
   - Topological semi-metals and nodal superconductors
Books and review articles

Review articles:
- Y. Ando and L. Fu, arXiv:1501.00531

Books:
1st lecture: Topological band theory

1. Introduction
   - What is topology?
   - Bloch theorem
   - Topological band theory

2. Topological insulators in 1D
   - Berry phase
   - Simple example: Two-level system
   - Polyacetylene (Su-Schrieffer-Heeger model)
   - Domain wall states
What is topology?

The study of geometric properties that are insensitive to smooth deformations

For example, consider two-dimensional surfaces in three-dimensional space

Closed surfaces are characterized by their genus \( g = \# \) holes

\[
g = 0.
\]

\[
g = 1
\]

Topological equivalence:

Two surfaces are equivalent if they can be continuously deformed into one another without cutting a hole.

topological equivalence classes distinguished by genus \( g \) (topological invariant)

Gauss-Bonnet Theorem

Genus can be expressed in terms of an integral of the Gauss curvature over the surface

\[
\int_S \kappa \, dA = 4\pi (1 - g)
\]
Band theory of solids and topology

**Bloch’s theorem:** consider electron wavefunction in periodic crystal potential

Electron wavefunction in crystal \( |\psi_n\rangle = e^{i\mathbf{k}\mathbf{r}} |u_n(\mathbf{k})\rangle \)

Bloch wavefunction has periodicity of potential

**Bloch Hamiltonian**
\[
H(\mathbf{k}) = e^{-i\mathbf{k}\mathbf{r}} H e^{+i\mathbf{k}\mathbf{r}}
\]

\( H(\mathbf{k}) |u_n(\mathbf{k})\rangle = E_n(\mathbf{k}) |u_n(\mathbf{k})\rangle \)

\( \mathbf{k} \in \text{Brillouin Zone} \)

Band structure defines a mapping:

Brillouin zone \( \xrightarrow{\quad} \quad H(\mathbf{k}) \quad \) Hamiltonians with energy gap

**Topological equivalence:**

Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap
**Topological band theory**

- Consider band structure with a gap:
  
  \[ H(k)|u_n(k)\rangle = E_n(k)|u_n(k)\rangle \]

  - *band insulator*: \( E_F \) between conduction and valence bands
  - *superconductor*: band structure of Bogoliubov quasiparticles

- **Topological equivalence:**
  
  Two band structures are equivalent if they can be continuously deformed into one another **without closing the energy gap** and **without breaking the symmetries** of the band structure.

- Symmetries to consider:
  
  - *particle-hole symmetry*, time-reversal symmetry
  - reflection symmetry, rotation symmetry, etc.

- Top. equivalence classes distinguished by:

  **topological invariant (e.g. Chern no):**

  \[ n_Z = \frac{i}{2\pi} \int \mathcal{F} \, dk \in \mathbb{Z} \]

  *Berry curvature*
Topological band theory

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**Bulk-boundary correspondence:**

\[ |n_{\mathbb{Z}}| = \# \text{ gapless edge states (or surface states)} \]
Band theory and topology

Berry phase:

Phase ambiguity of wavefunction \( |u(k)\rangle \rightarrow e^{i\phi_k} |u(k)\rangle \)

\(U(1)\) fiber bundle: to each \(k\) attach fiber \( \{ g |u(k)\rangle \mid g \in U(1) \} \)

define Berry connection: (like EM vector potential)

\[ \mathcal{A} = \langle u_k | -i \nabla_k | u_k \rangle \]

under gauge transformation:

\[ |u(k)\rangle \rightarrow e^{i\phi_k} |u(k)\rangle \quad \implies \quad \mathcal{A} \rightarrow \mathcal{A} + \nabla_k \phi_k \]

Berry phase: (gauge invariant quantity)

change in phase on a closed loop

\[ \gamma_C = \oint_C \mathcal{A} \cdot dk \]

Berry curvature tensor: (gauge independent)

\[ \mathcal{F}_{\mu\nu}(k) = \frac{\partial}{\partial k_\mu} \mathcal{A}_\nu(k) - \frac{\partial}{\partial k_\nu} \mathcal{A}_\mu(k) \]

For 3D: \( \mathcal{F} = \nabla_k \times \mathcal{A} \)

\[ \mathcal{F}_{\mu\nu} = \epsilon_{\mu\nu\xi} \mathcal{F}_\xi \]

Stokes:

\[ \gamma_C = \int_S \mathcal{F} \cdot dk \]

Topological invariants of band structures:

Topological property of insulating material given by Chern number (or winding number):

\[ n = \frac{i}{2\pi} \sum_{\text{filled states}} \int \mathcal{F} d^2k \]
Berry phase for two-band model

Two-level Hamiltonian:  \[ H(k) = d(k) \cdot \sigma = \begin{pmatrix} d_x - id_y & d_x + id_y \\ d_z & d_x + id_y & -d_z \end{pmatrix} \]

param. by spherical coord.: \[ d(k) = |d|(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \]

two eigenvectors with energies \[ E_{\pm} = \pm |d| \] (north pole gauge)

\[ |u_{k}^{-}\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix} \quad |u_{k}^{+}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix} \]

Berry vector potential: (gauge dependent)

\[ A_{\theta} = i \langle u_{k}^{-}\ | \partial_{\theta} \ | u_{k}^{-}\rangle = 0 \quad A_{\phi} = i \langle u_{k}^{-}\ | \partial_{\phi} \ | u_{k}^{-}\rangle = \sin^{2}(\theta/2) \]

Berry curvature: (gauge independent)

\[ \mathcal{F}_{\theta \phi} = \partial_{\theta} A_{\phi} - \partial_{\phi} A_{\theta} = \frac{\sin \theta}{2} \]

If \( d(k) \) depends on parameters \( k \):

\[ \mathcal{F}_{k_i, k_j} = \frac{\sin \theta}{2} \frac{\partial(\theta, \phi)}{\partial(k_i, k_j)} \]

Simple example: \( d(k) = k \)

\[ \mathcal{F} = \frac{1}{2} \frac{\hat{k}}{k^2} \] (monopole field)

\[ \gamma_C = \int_{S} \mathcal{F}_{\theta \phi} d\theta d\phi = \frac{1}{2} \left( \text{solid angle swept out by } \hat{d}(k) \right) \]
Polyacetylene (Su-Schrieffer-Heeger model)

Su-Schrieffer-Heeger model describes polyacetylene $[C_2H_2]_n$

Hamiltonian:

$$\mathcal{H} = \sum_i \left[ (t + \delta t) c_{A,i}^\dagger c_{B,i} + (t - \delta t) c_{A,i+1}^\dagger c_{B,i} + \text{h.c.} \right]$$

phonons lead to Peierls instability $\rightarrow$ finite $\delta t$

two degenerate ground states:

$\delta t > 0$

$\delta t < 0$

in momentum space:

$$\mathcal{H}(k) = d(k) \cdot \sigma = \begin{pmatrix} 0 & h(k) \\ h^\dagger(k) & 0 \end{pmatrix}$$

$$d_x(k) = (t + \delta t) + (t - \delta t) \cos k$$
$$d_y(k) = (t - \delta t) \sin k$$
$$d_z(k) = 0$$

Sublattice symmetry: $\sigma_z \mathcal{H}(k) + \mathcal{H}(k) \sigma_z = 0$ $\rightarrow$ $d_z = 0$ (energy spectrum is symmetric)

Energy spectrum:

$$E_{\pm} = \pm |d| = \pm \sqrt{2} \sqrt{t^2 + (\delta t)^2 + [t^2 - (\delta t)^2] \cos k}$$
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\]

\[
d_y(k) = (t - \delta t) \sin k
\]

Winding no: $\nu_1 = \frac{i}{2\pi} \int dk \ \text{Tr} \ [q^{-1} \partial_k q]$

\[
q(k) = \frac{h(k)}{|d(k)|}
\]

$\delta t > 0$:

Berry phase 0

$\nu_1 = 0$

$\delta t < 0$:

Berry phase $\pi$

$\nu_1 = 1$

Provided $d_z = 0$ (required by sublattice symmetry) states with $\delta t > 0$ and $\delta t < 0$ are topologically distinct
Domain Wall States in Polyacetylene

**Domain wall** between different topological states has topologically protected zero-energy modes

Effective low-energy continuum theory: (expand around $k_0 = \pi$)

$$H(x) = -i \sigma_y \partial_x + m(x) \sigma_x \quad m(x) = 2 \delta t$$

Dirac Hamiltonian with a mass:

$$E(q) = \pm \sqrt{q^2 + m^2}$$

Sublattice symmetry ("chiral symmetry"):

$$\{\sigma_z, H\} = 0 \quad \rightarrow \quad \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$$

Consider domain wall:

**Ansatz for boundstate:**

$$\psi_0 = \chi e^{-\int_0^x m(x') dx'}$$

$$H\psi_0 = 0 \Rightarrow \chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Bulk-boundary correspondence:

$$\Delta \nu = |\nu_R - \nu_L| = \# \text{ zero modes} \quad (\text{topological invariant characterizing domain wall})$$

[Su, Schreiffer, Heeger 79]
[Jackiw, Rebbi]