Modern Topics in Solid-State Theory: Topological insulators and superconductors

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Topological insulators and superconductors

1. Topological band theory
   - What is topology?
   - SSH model (polyacetylene)
   - Chern insulator and IQHE

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

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

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

Review articles:
- M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010)
- Y. Ando and L. Fu, arXiv:1501.00531
- E. Witten, arXiv:1510.07698

Books:
Lecture One: 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

3. Chern insulator and IQHE
   - Integer quantum Hall effect
   - Chern insulator on square lattice
   - Topological invariant
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 \( g = \# \text{ holes} \).

\[ g = 0. \]

\[ g = 1. \]

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 \( |\psi_n\rangle = e^{ikr} |u_n(k)\rangle \)  

**Bloch Hamiltonian** \( H(k) = e^{-ikr}He^{ikr} \) \( \implies H(k)|u_n(k)\rangle = E_n(k)|u_n(k)\rangle \)

\( k \in \) Brillouin Zone

Band structure defines a mapping:

Brillouin zone \( \longrightarrow H(k) \) 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:

\[ H(\mathbf{k}) \left| u_n(\mathbf{k}) \right\rangle = E_n(\mathbf{k}) \left| u_n(\mathbf{k}) \right\rangle \]

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

**Topological equivalence:**

Two band structures are equivalent if they can be continuously deformed into one another \textit{without closing the energy gap} and \textit{without breaking the symmetries} of the band structure.

\[ \uparrow \] symmetries to consider:

- \textit{particle-hole symmetry}, time-reversal symmetry
- reflection symmetry, rotation symmetry, etc.

\[ \uparrow \] top. equivalence classes distinguished by:

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

\[ \text{topological invariant (e.g. Chern no)} \]
Topological band theory

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**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): \( n_\mathbb{Z} = \frac{i}{2\pi} \int \mathcal{F} \, d\mathbf{k} \in \mathbb{Z} \)

**Bulk-boundary correspondence:**

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

**Berry phase:**

Phase ambiguity of wave function: 
\[ |u(k)\rangle \rightarrow e^{i\phi_k} |u(k)\rangle \]

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

define **Berry connection:** (like EM vector potential)

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

under gauge transformation:

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

**Berry phase:** (gauge invariant quantity)

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

change in phase on a closed loop

**Berry curvature tensor:** (gauge independent)

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

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):

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

**Two-level Hamiltonian:**

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

param. by spherical coord.: \( \mathbf{d}(\mathbf{k}) = |\mathbf{d}|(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \)

two eigenvectors with energies \( E_\pm = \pm |\mathbf{d}| \) (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)

\[
A_\theta = i \langle u^-_k | \partial_\theta | u^-_k \rangle = 0 \\
A_\phi = i \langle u^-_k | \partial_\phi | u^-_k \rangle = \sin^2(\theta/2)
\]

**Berry curvature:** (gauge independent)

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

If \( \mathbf{d}(\mathbf{k}) \) depends on parameters \( \mathbf{k} \):

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

**Simple example:** \( \mathbf{d}(\mathbf{k}) = \mathbf{k} \)

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

\[ \gamma_C = \int_S \mathcal{F}_{\theta\phi} \, d\theta d\phi = \frac{1}{2} \left( \frac{\text{solid angle}}{\text{swept out by } \hat{\mathbf{d}}(\mathbf{k})} \right) \]

\[ 2\gamma_C = \text{solid angle swept out by } \hat{\mathbf{d}}(\mathbf{k}) \]
Polyacetylene (Su-Schrieffer-Heeger model)

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

**Hamiltonian:**

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

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

Two degenerate ground states:

$\delta t > 0$

$\delta t < 0$

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

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

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

Energy spectrum: $E_{\pm} = \pm |\mathbf{d}| = \pm \sqrt{2} \sqrt{t^2 + (\delta t)^2 + [t^2 - (\delta t)^2] \cos k}$
Polyacetylene (Su-Schrieffer-Heeger model)

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

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

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

$$q(k) = \frac{|h(k)|}{|\mathbf{d}(k)|}$$  

$\mathbf{d}(k)$ is due to

$E_{\pm} = \pm |\mathbf{d}|$

$\delta t > 0$:

- 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 [Su, Schreiffer, Heeger 79]

zero-energy state at domain wall

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

$$H(x) = -i\sigma_y \partial_x + m(x)\sigma_x$$

$m(x) = 2\delta t$

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: 

zero-energy state at 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: 

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